Supporting Information for

Kinetics Tuning of Li-ion Diffusion in Layered $\text{Li}(\text{Ni}_x\text{Mn}_y\text{Co}_z)\text{O}_2$

Yi Wei^{1,†}, Jiaxin Zheng^{1,†}, Suihan Cui^{1,†}, Xiaohe Song¹, Yantao Su¹, Wenjun Deng¹,

Zhongzhen Wu¹, Xinwei Wang¹, WeiDong Wang³, Mumin Rao⁴, Yuan Lin¹,

Chongmin Wang⁴, Khalil Amine⁵, and Feng Pan^{1,*}

¹School of Advanced Materials, Peking University, Shenzhen Graduate School, Shenzhen

518055, People's Republic of China.

²Shenzhen Tianjiao Technology Development Co., Ltd., Shenzhen 518119, People's Republic

of China.

³Shenzhen OptimumNano Energy Co.,Ltd, Shenzhen 518118, People's Republic of China.

⁴Environmental Molecular Science Laboratory, Pacific Northwest National Laboratory, 902

Battelle Boulevard, Richland, Washington 99352, United States

⁵Electrochemical Technology Program, Chemical Sciences and Engineering Division,

Argonne National Laboratory, Argonne, IL 60439, United States

[†]These authors contributed equally to this work.

*Corresponding author: panfeng@pkusz.edu.cn

Ab initio computational details.

All calculations are performed using the plane-wave projector-augmented wave method¹, as implemented in the Vienna *ab initio* simulation package². The Perdew-Burke-Ernzerhof (PBE)³ form of generalized gradient approximation (GGA) is chosen as the exchange-correlation potential. Structural properties and electronic properties are calculated by the PBE+*U* approach⁴ with spin polarization, with *U* values of Mn, Co, and Ni being set as 3.5 eV, 3.3 eV, and 6.4 eV, respectively. These *U* values are adopted according to the simulation parameters of Li(Ni_xMn_yCo_z)O₂ models from the Materials Project website (www.materialsproject.org). The calculated lattice parameters using these *U* values for all the samples are very close to the experimental lattice parameters (Table S1). In addition, these *U* values have also been tested to calculate the voltage profiles of Li extraction for (532) and (622), which also agree well with the experimental results (Fig. S4). Climbing-image nudged elastic band (cNEB) method is applied in this work to calculate the activation energy of the Li hopping between two sites⁵.

All the structures in this work are layered structure with space group $R\bar{3}m$, as α -NaFeO₂ model. The cut-off energy for plane wave is 450 eV⁶. K-points for sampling in Brillouin zone are between $4 \times 4 \times 2$ and $6 \times 6 \times 2$ according to the scale of the reciprocal lattice in our first-principle calculation models. Molecular dynamics and activation barrier calculation are performed in supercells: LiCoO₂, LiMnO₂, LiNiO₂ and LiNi_{0.33}Mn_{0.33}Co_{0.33}O₂ are $3 \times 3 \times 1$; LiNi_{0.42}Mn_{0.42}Co_{0.16}O₂ is $4 \times 3 \times 1$ ⁶, and LiNi_{0.5}Mn_{0.3}Co_{0.2}O₂ is $5 \times 2 \times 1$. Therefore, the composition of Ni, Co, and Mn is

approximately equal in each single layer. Besides, large lattice also isolates each atom in the period structure and ensures their dynamics movement. Otherwise, $1 \times 1 \times 1$ lattice would force all atoms in one single layer to move in the same direction. The arrangement of Ni, Co, and Mn atoms would affect the total energy of the cell and it has a relatively large possibility of arrangement in 333, 442, 532 etc. Here we adopt a simplified model, in which the transition metal atoms are arranged with certain ordering in the compounds⁶. After cell parameters are fully relaxed and optimized, which also agree well with the experimental results and previous theoretical results (Table S1). We calculated the total energies of three different transition metal ordering models and found that the most energetically favorable structure is the one shown in Fig. S1 – S3. These materials are applied with antiferromagnetic structure to reach the minimum energy instead of other magnetic structures, consistent with previous report⁷.

As a result of diffusion between lithium ions positions, the diffusion coefficient depends on the barrier energy between two lithium ion sites:

$$D_l = D_0 e^{-\frac{E_a}{kT}}, \quad (1)$$

where E_a is the activation energy, D_0 is the diffusion constant, and D_l is the diffusion coefficient. Activation barriers for lithium migration in different lithium vacancy environments were calculated with the first-principles pseudo-potential method with the GGA level. The activation barrier of lithium in oxide system is actually not sensitively dependent on the choice of either LDA or GGA⁸. In this research, the climbed nudged elastic band method (cNEB), as modification to NEB, has been used

to study the energy barriers⁹ in supercell $3 \times 3 \times 1$ with 5 images as intermediate states. These intermediate images are optimized along the diffusion path and each image is relaxed to its favorable energy, constrained by certain ratio of energy difference and distance to neighboring images. Large supercell ensures that each hopping atoms are isolated from their periodic images, providing an accurate energy barrier in dilute limit (the images of migrating Li are more than 6 Å apart). All activation barriers are performed in the dilute vacancy limit with 26 Li and 1 vacancy in the cell, that means the only vacancy in 27 Li position affects the whole lattice very little after taking a Li atom away from it. Ni²⁺, Ni³⁺, Co³⁺, and Mn⁴⁺ are obtained in lithiated states of 552, LiNiO₂, LiCoO₂, and 552, respectively. Ni⁴⁺ is obtained in delithiated LiNiO₂.

We calculated the diffusion coefficients for all materials mentioned above by the ab initio molecule dynamics (MD) method also implemented in VASP. The diffusion coefficient is calculated as the averaged mean square displacement of Li atoms over time. We simulated the thermal motion of the atoms in lattice for 6 ps with 3 fs time step in MD simulation. MSD analysis can help us to find the MSD vs. time through the data from MD simulation. MSD of single molecule is given down below:

$$MSD_i = (x_i^2 + y_i^2 + z_i^2) - (x_0^2 + y_0^2 + z_0^2) \quad (2)$$

where x_i , y_i , and z_i refer to the current position of atoms and x_0 , y_0 , z_0 stand for the original site of atoms. In first-principle MD simulations, atoms barely move in room temperature. So we raised the temperature to 500 K to make them diffuse. According to Eq. 1, $\log(D_i)$ is linear to $1 / T$. After getting these diffusion coefficient data in

high temperature, we perform linear fitting to reach the diffusion coefficient at room temperature, which makes it comparable to those data obtained in experiments.

Experiments details.

The series of layered compounds $\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$ were synthesized by the co-precipitation method followed by solid-state reaction as described elsewhere.¹⁰ A 5% excess of lithium was added to make sure that the molar ratio for $\text{Li} / (\text{Ni} + \text{Mn} + \text{Co})$ is around unity. The final sintering procedure was done at 800 °C for 8 h and then the sample was quenched to room temperature by sandwiching it between two copper plates. The synthesis conditions for the four compositions were exactly the same. A temperature of 900 °C was used to prepare pellets for density measurements.

Experiments were performed using electrochemical cells consisting of positive electrode made of NCM, negative electrode made of metal Li and electrolyte made of EC: DEC. These NCM materials include the $\text{Li}(\text{Ni}_{0.33}\text{Mn}_{0.33}\text{Co}_{0.33})\text{O}_2$, $\text{Li}(\text{Ni}_{0.4}\text{Mn}_{0.4}\text{Co}_{0.2})\text{O}_2$, $\text{Li}(\text{Ni}_{0.42}\text{Mn}_{0.42}\text{Co}_{0.16})\text{O}_2$, $\text{Li}(\text{Ni}_{0.5}\text{Mn}_{0.3}\text{Co}_{0.2})\text{O}_2$, $\text{Li}(\text{Ni}_{0.6}\text{Mn}_{0.2}\text{Co}_{0.2})\text{O}_2$ and $\text{Li}(\text{Ni}_{0.7}\text{Mn}_{0.15}\text{Co}_{0.15})\text{O}_2$. To measure the Li-ion diffusion coefficient, we used the GITT method which is widely used, as shown in Fig. S4 and S5. All the cells were discharged at 0.05 C for 15 minutes, and rest for 45 minutes repeatedly from 4.35 V to 3.3 V. The experiments were performed at 25 °C (298 K).

The cell is subjected to a small constant current, and the potential changes are measured as a function of time. One important assumption is that the diffusion in the solid solution electrode (NCM) is one-dimensional diffusion.¹¹ And we don't take the

ohmic potential drop, double-layer charging, charge-transfer kinetics and phase transformation into consideration.^{11a} Then the Li-ion diffusion coefficient can be calculated by Fick's law through the following equation.¹²

$$D_s = \frac{4}{\pi} \left(\frac{IV_M}{z_A FS} \right) \left[\frac{(dV(x)/dx)}{(dV(t)/d\sqrt{t})} \right]^2 \quad (t \ll L^2/D_s) \quad (3)$$

Where F (C/mol) is the Faraday constant ($F = 96485.3$ C/mol), z_A is the charge number of the active material (for the Li-ion batteries, $z_A = 1$), S (cm²) is the interfacial area between the electrode and the electrolyte of the cell, I (A) is the applied current which is constant during the current pulse, and V_M (cm³/mol) is the molar volume of the active material. Besides, we can measure the value of $dV(t)/d\sqrt{t}$ and $dV(x)/dx$ by plotting the voltage against the square root of the time during constant current pulse and the equilibrium electrode voltage against the SOC (State of Charge) after each current pulse, respectively. For the NCM electrode, we assume that the solid phase is consisted of spherical particles with radius R_s .^{11b} And the applied current was very small for the cells.^{12b} So the Eq.3 becomes

$$D_s = \frac{4}{\pi\tau} \left(\frac{R_s}{3} \right)^2 \left(\frac{\Delta V_s}{\Delta V_t} \right)^2 \quad (4)$$

Where τ (s) is the time duration of the pulse. While ΔV_s and ΔV_t can be calculated in Fig. S5 and S6. Then D_s can be calculated.

After activated, all the cells were charged to 4.35 V, and rest until the voltage was stable. We used MACCOR (Model MC-16 Battery Test System, 5 V, 5 A) to perform

the GITT experiments. The cells were test in the thermotank (RKS-80L, 220 V) to keep the temperature constant.

Because of the assumptions, there are some errors. The particles are not completely uniform, but for the same kind of material, the errors caused by R_s are same. Another error caused by ΔV_s is mainly because of the unbalanced voltage after rest for 45 minutes when $0 < x < 0.15$ and meanwhile, the assumption of GITT that $t \ll L^2/D_s$ is no longer valid out of the range mentioned above.^{11b}

The difference in the diffusion coefficients between the calculation values and the experimental results.

There is a difference of nearly two orders of magnitude in the diffusion coefficients between the calculation values and the experimental results ($\sim 10^{-9}$ cm²/S for calculations and $\sim 10^{-11}$ cm²/S for experiments). We mainly attribute this difference of two orders of magnitude in the diffusion coefficients to errors of the experimental measurements. Due to the factors such as the inaccuracy of the assumptions, the distribution of the NMC particle size, the jitter of the cell voltage, and so on, the GITT measurement has its model errors. For example, the size of the NMC particles is heterogeneous, so it has a distribution. According to Eq. 4, the error in spherical particles radius R_s affects D_s . Usually, R_s is smaller than actual radius. Besides, at the beginning and ending of the discharge, the voltage is unbalanced after 30 minutes rest. Despite these errors, no better method than GITT has been developed. As a result, previous studies reported that diffusion coefficient for NMC materials is usually in the

range of 10^{-8} and 10^{-11} cm^2/S in GITT and PITT test ¹³.

Comparison of the diffusion properties obtained by ab initio MD and cNEB methods.

In this work, the diffusion coefficient (D_s) is calculated as the averaged mean square displacement of Li atoms over time from the ab initio MD in VASP, and we get the D_s at room temperature (300 K) through an Arrhenius linear fitting the D_s values at high temperatures, according to $D_s = D_0 e^{-\frac{E_{\text{eff}}}{kT}}$. Meanwhile, we can get the E_{eff} by extracting the slope of the linear fitting, which is in the range of 170 – 200 meV at SOC = 1/3. The activation barriers calculated by cNEB method are 357 meV for Ni^{2+} and 429 meV for Ni^{3+} , respectively, larger than the E_{eff} at SOC = 1/3 by ab initio MD method. This difference can be attributed to that E_{eff} obtained by ab initio MD method is a mean and statistical effective activation energy for all diffusion pathways. The Li slab space expands at SOC = 1/3, which would reduce the effective activation barrier. Moreover, as the E_{eff} is obtained by linearly fitting the D_s values at high temperatures, the fitting errors and volume effect also contribute to the difference. By contrast, cNEB method is used to calculate the migration barrier at ground state, and the barrier reflects the activation energy of the electrostatic interaction contribution for Li-ion diffusion along a specific pathway. In addition, the strain effect (Li slab space) during delithation is not considered in cNEB method.

Suggestions about the recent hot Li_2MnO_3 -based oxides.

Finally, according to our calculations, the activation barrier of Li-ion diffusion near Mn^{4+} is as high as 0.91 eV for ODH route and 0.523 eV for TSH route, respectively. It is hard for Li-ion diffusion in recent hot layered Li_2MnO_3 -based oxides¹⁴, because the Mn is in its +4 valence state. This is also one of the reasons accounting for the electrochemical inactive property for such Li_2MnO_3 -based oxides. Lowering the valence state of partial Mn and doping Ni (Ni^{2+} and Ni^{3+}) could introduce some advance diffusion channels for Li-ion diffusion, which would improve the electrochemical activity. Reported studies demonstrated that removal of Li_2O from such Li_2MnO_3 -based oxides can leaves an electrochemically active layered MnO_2 component for lithiation and delithiation. Therefore, lower valence states for Mn can also be induced after lithiation, which would facilitate the Li-ion diffusion.

Table S1. A comparison of the calculated lattice parameters in different layered materials with the reported calculation and experimental results.

Compound		Lattice Parameter			
		a(Å)	c(Å)	c/a	V(Å ³)
LiCoO ₂	our work	2.8045	13.7496	4.9026	93.6579
	other cal. ¹⁵	2.8130	13.5900	4.8311	93.1300
	Exp. ¹⁶	2.8140	14.0440	4.9908	96.3096
LiNiO ₂	our work	2.7833	13.6881	4.9180	91.8288
	other cal. ¹⁵	2.8370	13.7100	4.8326	95.5623
	Exp. ¹⁶	2.8800	14.1870	4.9260	101.9075
LiMnO ₂	our work	2.9124	14.5136	4.9834	106.6121
	other cal. ¹⁵	2.9320	14.1600	4.8295	105.4197
	our work	2.8419	13.9905	4.9229	97.8550
333	other cal. 1 ¹⁵	2.8310	13.8800	4.9029	96.3385
	other cal. 2 ¹⁵	2.8270	13.9400	4.9310	96.4817
	Exp. ¹⁷	2.8670	14.2460	4.9690	101.4096
442	Our work	2.8412	14.1142	4.9676	98.6712
	Exp. ¹⁸	2.8694	14.2661	4.9719	101.7227
532	our work	2.9216	14.2976	4.8937	105.6920
	Exp. ¹⁹	2.8720	14.2410	4.9586	101.7279
552	our work	2.8914	14.0570	4.8617	101.7741
	Exp. 1 ⁶	2.8812	14.2950	4.9615	102.7689
	Exp. 2 ⁶	2.8946	14.3801	4.9679	104.3467
622	Our work	2.8935	14.3548	4.9610	104.0835
	Exp. 1 ²⁰	2.8750	14.2310	4.9499	101.8689
	Exp. 2 ²¹	2.8714	14.2191	4.9520	101.5290
811	Our work	2.8788	14.3028	4.9529	103.2961
	Exp. ²²	2.8771	14.2460	4.9515	102.1253

Table S2. The ratio of $\text{Ni}^{2+}/\text{Ni}^{3+}/\text{Ni}^{4+}$ in different materials at different SOC.

SOC	0	0.33	0.5
333	0.33/0/0	0/0.33/0	0/0.17/0.33
442	0.4/0/0	0.07/0.33/0	0/0.3/0.1
552	0.42/0/0	0.09/0.33/0	0/0.34/0.08
550	0.5/0/0	0.17/0.33/0	0/0.5/0
532	0.3/0.2/0	0/0.47/0.03	0/0.3/0.2
622	0.2/0.4/0	0/0.47/0.13	0/0.3/0.3
71515	0.15/0.55/0	0/0.52/0.18	0/0.35/0.35
811	0.1/0.7/0	0/0.57/0.23	0/0.4/0.4

Table S3. Calculated average Li slab space of different NMC materials at (a) SOC = 0;
(b) SOC = 0.5.

(a)

NMC	333	442	552	550	532	622	71515	811	LiNiO ₂
Li slab (Å)	2.624	2.614	2.610	2.613	2.612	2.701	2.553	2.527	2.510

(b)

NMC	333	552	532
Li slab (Å)	2.650	2.684	2.719

Table S4. Ionic radius of transition metal ions (low spin state).

Ion	Mn ⁴⁺	Co ³⁺	Ni ²⁺	Ni ³⁺	Ni ⁴⁺
Ionic radius (pm)	53	54.5	69	60	48

Figure S1. Different models for the cation ordering of transitional metal layer in (552) adopted in the calculation and the corresponding calculated total energies.

Figure S2. Different models for the cation ordering of transitional metal layer in (333) adopted in the calculation and the corresponding calculated total energies.

Figure S3. Different models for the cation ordering of transitional metal layer in (442) adopted in the calculation and the corresponding calculated total energies.

Figure S4. Experimental and calculated voltage profiles of Li extraction for (532) and (622).

Figure S5. GITT data for a NCM333 coin cell. The cell was discharged at 0.05 C for 15 minutes, and rest for 45 minutes at room temperature (25 °C) in the thermostatic tank repeatedly until the voltage was less than 3.3 V. (a) Current vs Time, (b) Voltage vs Time.

Figure S6. Zoomed-in voltage corresponding to box in Fig. S4 (b). The red line divides the figure into two parts. The left part stands for the discharge pulse, while the right part stands for the rest step.

Figure S7. Arrhenius plot of diffusion coefficient (D_s) at SOC = 1/3.

Figure S8. Variation of the chemical diffusion coefficient, D_{Li^+} in GITT test, including 333, 442, 622, and two samples of 532. Data points between $x = 0.15$ and $x = 0.5$ are accuracy enough. The error of data points in $x = 0.05 - 0.15$ is about 10 %, but the trend of those data is still reliable.

Figure S9. A map of relationship between nickel content in $\text{Li}(\text{Ni}_x\text{Co}_y\text{Mn}_z)\text{O}_2$ and diffusion coefficient at SOC = 1/3. Color of the dot refer to the nickel's valence ratio of this material at SOC = 1/3.

**Geometrical coordinates and total energies of all the optimized and most energy
stable structures.**

LiCoO₂

1.0000000000000000		
2.4401865750657512	-1.4088423759871218	0.0000000000000000
0.0000000000000000	2.8176847519742436	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.7495867080420643

Li	O	Co
3	6	3

Direct

0.6666666666666643	0.3333333333333357	0.3333399871220898
0.3333333333333357	0.66666666666666714	0.6666600128779102
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.3333333333333357	0.66666666666666714	0.4256200112769801
0.0000000000000000	0.0000000000000000	0.7589450782910813
0.0000000000000000	0.0000000000000000	0.2410549217089190
0.33333333333333286	0.66666666666666714	0.9077138785465503
0.6666666666666643	0.3333333333333357	0.0922861214534498
0.66666666666666714	0.33333333333333286	0.5743799887230197
0.6666666666666643	0.3333333333333357	0.8333313610464999
0.3333333333333357	0.66666666666666714	0.1666686389535000
0.0000000000000000	0.0000000000000000	0.5000000000000000

E₀ = -74.406583 eV

LiNiO₂

1.0000000000000000

2.4616872764440543	-1.4212558117156500	0.0000000000000000
0.0000000000000000	2.7833116234312999	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.6881730431539528

Li	O	Ni
3	6	3

Direct

0.6666666666666643	0.3333333333333357	0.3333224407531228
0.3333333333333357	0.66666666666666714	0.6666775592468772
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.3333333333333357	0.66666666666666714	0.4235494348021467
0.0000000000000000	0.0000000000000000	0.7568854206838669
0.0000000000000000	0.0000000000000000	0.2431145793161331
0.3333333333333286	0.66666666666666714	0.9097871940893242
0.6666666666666643	0.3333333333333357	0.0902128059106758
0.66666666666666714	0.3333333333333286	0.5764505651978531
0.6666666666666643	0.3333333333333357	0.8333359609977470
0.3333333333333357	0.66666666666666714	0.1666640390022530
0.0000000000000000	0.0000000000000000	0.5000000000000000

E₀ = -67.020909 eV

LiMnO₂

1.0000000000000000

2.4557793257479870	-1.4178448547909162	0.0000000000000000
0.0000000000000000	2.9124897095818323	0.0000000000000000
0.0000000000000001	0.0000000000000000	14.5135740068612254

Li	O	Mn
3	6	3

Direct

0.6666666666666643	0.3333333333333357	0.3332902173453622
0.3333333333333357	0.66666666666666714	0.6667097826546377
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.3333333333333357	0.66666666666666714	0.4238047212232672
0.0000000000000000	0.0000000000000000	0.7571781483199730
0.0000000000000000	0.0000000000000000	0.2428218516800268
0.3333333333333286	0.66666666666666714	0.9095444372693652
0.6666666666666643	0.3333333333333357	0.0904555627306349
0.66666666666666714	0.3333333333333286	0.5761952787767328
0.6666666666666643	0.3333333333333357	0.8333180915750986
0.3333333333333357	0.66666666666666714	0.1666819084249014
0.0000000000000000	0.0000000000000000	0.5000000000000000

E₀ = -84.141042 eV

(333)

1.0000000000000000

2.4578332723966834	-1.4190366208586578	-0.0000001580989243
-0.0000052955475060	2.8419640705149838	0.0000006202844520
0.0000008225093822	0.0000030998148148	13.9905442132403936

Li	O	Mn	Co	Ni
3	6	1	1	1

Direct

0.6666666069125745	0.3333336596949383	0.3337707659133783
0.3333340196833458	0.6666654650039870	0.6593572539749597
-0.0000010413147236	0.0000016703913165	0.0070717424099547
0.3333356836331837	0.6666642414648374	0.4214452677697590
0.0000000982846711	0.0000003633643729	0.7588878992404079
0.0000000090090276	-0.0000005973424089	0.2382588890894988
0.3333336645981668	0.6666673150854274	0.9118585841940164
0.6666668306632066	0.3333327377689024	0.0933709463030478
0.6666642448968162	0.3333354926689798	0.5760453226143208
0.6666668975189869	0.3333338102080507	0.8348428054360695
0.3333331080232959	0.6666658586433624	0.1670384110704357
-0.0000001219085518	-0.0000000169517448	0.4980521119841511

$E_0 = -75.618608$ eV

(442)

1.000000000000000

5.6863139579760675 0.6673742246737236 0.0010219743976228

0.0278549942428520 12.4385067711748665 0.0119691193472298

0.0009339908891865 0.0135403174829620 14.1142969257961755

Li O Mn Co Ni

30 60 12 6 12

Direct

0.9567913438301627 0.1368559640113589 0.3336574221951322

0.7300433202761800 0.0700157241270588 0.6660581136326386

-0.0084399423367685 0.0018566666911350 -0.0000317995788234

0.1610701415361087 0.3395922073578303 0.3363102888199557

0.9296808400748913 0.2716849347594467 0.6678684019416514

0.2035798414829957 0.2069542059477704 -0.0061686562267206

0.3670169674048059 0.5342170833723916 0.3326348963991494

0.1286326628249164 0.4627234772526086 0.6646192699984842

0.4013122038131758 0.3990771528991352 -0.0022999511368905

0.5747215819065591 0.7276359730570802 0.3286715300044876

0.3367999831172804 0.6620656650897512 0.6633677327533278

0.5985877512978918 0.5980103562280937 0.0063932165836675

0.7604086411645309 0.9307898304277221 0.3329554391941895

0.5388394465212311 0.8663818690510066 0.6669873573640561

0.7930084290925122 0.7980838275980671 0.0023142638666483

0.4685342314724251 0.1349248879576602 0.3327429796706831

0.2315615477884332 0.0708657924671026 0.6684764979108463

0.5131714271030530 -0.0003247871778150 -0.0023918552311706

0.6721923218721785 0.3372678963321043 0.3344994179418692

0.4378915195890926 0.2704318905115772 0.6669695178860321

0.6949408369419667 0.2028196031942228 -0.0051742562076046

0.8675596347802489 0.5338119912553005 0.3319739191893364

0.6402685319475244 0.4607024562859794 0.6638856830220500

0.8974191928685410 0.4006051544288669 -0.0032734710673322

0.0639933289534261 0.7292293755171890 0.3322268172695723

0.8337461807022238 0.6632065525864665 0.6653238609093943

0.1027564330046922 0.5969265236321922 0.0026085874797593

0.2683776471353715 0.9304884078123727 0.3324083212949912

0.0252045623590645 0.8688302381032844 0.6635163418466851

0.3103478765043375 0.7968733372847715 0.0039927972584114

0.7205516484454327 0.0607297229610485 0.4194514112381675

0.0095017484454286 0.0018839393352338 0.7563324333820918

-0.0027110396996303 0.0020370867741235 0.2407079208411771

0.7444769680501383 0.0692669182593635 0.9118134432004722

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Li O Mn Co Ni

36 72 15 6 15

Direct

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Li	O	Mn	Co	Ni
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Direct

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0.9357519198417008	0.6674634273820745	0.3327358231599913
0.8640945245015956	0.8280976724445744	0.6645065703596317
0.7978962436744519	0.4976719098976858	-0.0000500600944741
0.0653187721586867	0.3219833275647548	0.4230526555552801
-0.0014780971378915	0.0058849166738775	0.7515083622057638
-0.0002512975058340	0.0095157169878612	0.2406146636851694
0.0649152715680315	0.3200332785668506	0.9073577099467582
0.1321211968676108	0.1779742989344408	0.0915365143628723
0.1310368673808373	0.1591853782500357	0.5728646527643739

0.2697508337863828	0.3326519854375765	0.4246771024639138
0.1958915729505050	-0.0094573620631284	0.7581272634889967
0.2038704593393674	0.0090679512848432	0.2406944388157316
0.2596953661535643	0.3263714920307587	0.9066005864109054
0.3308877531804618	0.1718057935866979	0.0844667609508337
0.3334110349265582	0.1768234306501581	0.5744295237005358
0.4660302528130759	0.3453947372845243	0.4247422283904385
0.3999690038064765	-0.0097725006769587	0.7579625967292877
0.4013097559915003	-0.0066726300616003	0.2475532363731480
0.4670914517908843	0.3248770558820949	0.9070701128672617
0.5269546353183510	0.1556264864690304	0.0911258063729282
0.5379833135410549	0.1763851873085316	0.5740627035302579
0.6643922265108907	0.3372358148175156	0.4171959226885552
0.6022177914626744	0.0061552550968810	0.7594116172945287
0.6016561047307237	-0.0116618511264627	0.2403858987028314
0.6673780947540903	0.3333993989855483	0.9073384279595346
0.7318264073158665	0.1563172881254044	0.0900342934711212
0.7349469524768721	0.1599227152115819	0.5804772885817947
0.8599344747441983	0.3225767197996282	0.4234199514129177
0.7984099577280176	0.0114570309184573	0.7580768998030475
0.7979692034310566	-0.0059983151362141	0.2397584837558633
0.8691920267867237	0.3587859643023779	0.9080560224625300
0.9365143505228843	0.1662019741864433	0.0913674752305313
0.9350828800594935	0.1551546673353344	0.5738887003048224
0.0659351642084062	0.8329174245866253	0.4245662888763563
0.0020209729611366	0.5151856369225909	0.7568505388535945
0.0014062653501154	0.5006872522783098	0.2416066953577149
0.0691484661910064	0.8282943917929179	0.9146572665807092
0.1402031358739527	0.6732662935646169	0.0924208184571605
0.1345591843950750	0.6789837259726599	0.5736549937179084
0.2665748288905552	0.8424598564020830	0.4251840205562774
0.1985719016792707	0.4750998241895230	0.7573195807521681
0.2015600580268549	0.5252052336416370	0.2413568887922750
0.2677128037341871	0.8215750986831676	0.9074705772939985
0.3349922242655644	0.6801865206775543	0.0913023293928210
0.3353468967585098	0.6685313445789247	0.5744797821391712
0.4737052775869803	0.8397763061478850	0.4254404171115617
0.3984311822557552	0.4983923293257786	0.7577447022908416
0.3980533932768039	0.4856412049215481	0.2412178420749982
0.4635768938202637	0.8331920268339188	0.9075372778718714
0.5311168516667197	0.6411464424163514	0.0906389312456158
0.5349776781849089	0.6916381466725156	0.5747861782815316
0.6687306846623690	0.8470037174193308	0.4243502378757332
0.5988124191614179	0.4874326607885162	0.7583476470872830

0.5930502157475996	0.4891051345710548	0.2391846153610334
0.6684664703805201	0.8439775922073151	0.9089932524777570
0.7325291147773946	0.6666111724841962	0.0913621062725756
0.7314677987744740	0.6507590111867196	0.5751989972655961
0.8644907683688486	0.8086639732330835	0.4240452718364540
0.8067766750657434	0.5113064871504764	0.7599576919239406
0.8007208035965578	0.5131632653499818	0.2400457056017666
0.8730993038417435	0.8441852784345927	0.9079347775988111
0.9328588407149447	0.6744693937624047	0.0918669597258013
0.9263739367528833	0.6541948689798777	0.5719837809246400
0.1214048489888069	0.1336940518618353	0.8318831161096880
0.2004314156071275	0.0006852280465345	0.5014815962558060
0.5329589752547739	0.1652734475825041	0.8308805085511154
0.4550518069224727	0.3006277643646948	0.1643993737316894
0.6119073946979180	0.0324962575343641	0.5004054643605768
0.2784455495612323	0.8662081207942993	0.1673486997326705
0.9449046603721972	0.6995904485432595	0.8348980272247432
0.8668449013039571	0.8345701343376223	0.1684305285677981
0.7884879963562974	0.4665060173368732	0.4974204382384961
0.0686376544741002	0.3432681412405634	0.1668386336959240
-0.0020701601185280	-0.0094008502580227	0.4984476595348690
0.7355607657492687	0.1756921129165801	0.8338322584724555
0.3311599090386379	0.6564101999103595	0.8322667053982316
0.4023014910145287	0.5099631236368065	0.4999560421927213
0.6644722393713388	0.8241752601452046	0.1649491970346580
0.3309353339909434	0.1591305251731802	0.8326589459376027
0.2654652956161292	0.3434887918073548	0.1655795446520306
0.4026789142109612	0.0078903745485721	0.4995995398153489
0.6645232757269143	0.3268706233748406	0.1657043417430295
0.9323078280072961	0.1766917405186667	0.8319749179147302
0.8658699068487866	0.3330123911988372	0.1661575852508946
0.8012228684668427	-0.0097963135842352	0.5000257930170540
0.1343978947827471	0.6566059467804963	0.8332601045331962
0.0689181934284382	0.8407493755594377	0.1665282755057845
-0.0021526842299570	0.4922440708017254	0.4987250037311038
0.1996895001830088	0.4993016207200843	0.4993286760846236
0.5340786167138938	0.6671611271527894	0.8330112526080661
0.4676120769746334	0.8229401473014125	0.1666755554492651
0.7356225494402362	0.6739174543982740	0.8332538377662557
0.5991672195023471	0.5100584406962915	0.4992061273654363

$E_0 = -681.06112 \text{ eV}$

(550)

1.0000000000000000

5.7412414791213422	-0.0365115315209697	-0.0383882459412300
-2.9021486767134768	4.9501624448305774	0.0448651468938971
-0.0928317169722556	0.0720884171859254	13.9711271542931321

Li	O	Mn	Ni
8	24	6	6

Direct

0.6677955308401293	0.3301848789187429	0.6653515667467044
0.5018297443236118	0.9979686188724259	0.9991981777474762
0.3314504255744511	0.6640796139141225	0.3343624245493262
0.1651470512275144	0.8362353804048311	0.6657421310710090
0.0013184361804471	0.4972566831894388	0.0012934060136033
0.8318210646917513	0.6690056036576997	0.3358036122107763
0.6666701198759328	0.8331489812813676	0.6635563870738000
0.4975846466104991	0.4971854542748951	-0.0003009301948049
0.1779694876745847	0.3570024091657559	0.4309520338198753
0.0029892151006508	0.9877711771549076	0.7591848463399642
0.9845031399619812	0.0025913415538576	0.2411870534032665
0.1873141961271060	0.3474949712171407	0.9047951574010158
0.3302502976361939	0.1689177687816765	0.0968647360058427
0.3505950552659468	0.1657801768937886	0.5700568304764368
0.6864257064566613	0.3359654031548830	0.4235898724203826
0.4833944714783373	-0.0013993106509913	0.7581198939701675
0.4901354267808348	0.9769851018100086	0.2358021357576238
0.6576533573943261	0.3360376290199107	0.9130322283886159
0.8403533294184616	0.1667527774627472	0.0912989338171863
0.8168654804118856	0.1644516468494076	0.5746321522985280
0.1659051856593279	0.8171227986536284	0.4227885713425004
-0.0003459242010742	0.5211934435656536	0.7615137969116111
0.0189237204589712	0.5120984129843960	0.2387464282884597
0.1629251864335955	0.8440593635845580	0.9115813856053113
0.3402043626646473	0.6530887495669061	0.0864769632196960
0.3315338409176256	0.6892046639099456	0.5768198653038489
0.6484784104217698	0.8173709567483517	0.4265037274888477
0.5194493224970350	0.4931127464305119	0.7570774366956265
0.4948507494205744	0.5153872747693088	0.2428878948724573
0.6487324427330619	0.8132681755241444	0.9061175753868639
0.8324479461590878	0.6668708659146678	0.0952196984870159
0.8291854016244901	0.6545661572575013	0.5757225096061396
0.3307266984662529	0.1677950650129078	0.8335372903572851
0.1651028651793707	0.3291098542168633	0.1689776853545372
0.5015314619420422	0.0034094629296775	0.4936552449373600
0.0023632906763742	0.4983738916558720	0.5018293649233063

0.8346129329950546	0.6693948400723161	0.8370581108369187
0.6686756905486054	0.8348882468564837	0.1646434377305077
0.0012457090559412	0.0023294590970622	0.4968631963939514
0.8347903710437752	0.1670451939924333	0.8335813309412619
0.6657781195867983	0.3311146132519202	0.1735994763491792
0.3319196305888969	0.6665163184374903	0.8298452475452638
0.1664830621578003	0.8338640147811247	0.1650702576905756
0.4992233429386845	0.4986190278596410	0.5020406204146944

$E_0 = -260.31631 \text{ eV}$

(622)

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6.0496851695169767	0.7872377609569569	-0.0953991808001466
0.2960247708243081	12.3413434428796158	-0.3892609568338122
-0.1795875968168933	-0.4406871155833331	14.3547918246666526

Li	O	Mn	Co	Ni
30	60	6	6	18

Direct

0.9636739238279880	0.1342685673027681	0.3308273864120271
0.7371887496123296	0.0677437329999909	0.6649096799641441
-0.0028773404374613	-0.0029066339318193	0.0047110430333513
0.1614478531104191	0.3328197228069933	0.3350852020268121
0.9375186501921233	0.2687835374079838	0.6622557028226025
0.1925367350213117	0.2020873889296631	-0.0022927976597561
0.3682638512188607	0.5329598557596539	0.3327555606984464
0.1332225470945309	0.4670670592282378	0.6667101933141494
0.3978127611055220	0.4032414525849933	-0.0023993861517984
0.5690051967461742	0.7339444677482434	0.3315695513600980
0.3352980842635700	0.6660444364105754	0.6682757305874499
0.6006149777617024	0.5999371114254360	-0.0046568370708564
0.7705936095270727	0.9320255569874919	0.3295754123340263
0.5415822951299144	0.8670752921897055	0.6636387809183035
0.8011323222995447	0.8009026888314406	-0.0006647863872314
0.4674251661507714	0.1327830856755883	0.3323617883868266
0.2302937615861364	0.0689847994084177	0.6616176628167080
0.5036937553202834	-0.0027060904248815	0.0049738686078891
0.6715748966382831	0.3319585566796310	0.3354410203441632
0.4285121148468448	0.2699514390025361	0.6602548826033409
0.7049130165862388	0.1992403103570855	0.0020837069875587
0.8632420916491881	0.5320497480004457	0.3328839842677493
0.6345285112262548	0.4684989883959217	0.6642666693777571
0.9036404368648223	0.4004468670216876	0.0003221379913154
0.0654420762002541	0.7355997757683814	0.3329573265315993
0.8329733859111031	0.6679205937270254	0.6665185174581322
0.0983612054568459	0.6016386311777545	-0.0045386140004009
0.2624918251233296	0.9310187398977476	0.3291570098463206
0.0274059586296571	0.8651548120956902	0.6644509715539355
0.3004798779411190	0.8002269062171231	0.0033063105275881
0.7467448469965207	0.0664388046051551	0.4269220569882438
0.0024852165168829	-0.0031592330235507	0.7601919453239550
-0.0034350079616047	0.0036507348621303	0.2389600394589380
0.7417751778062325	0.0697765477497491	0.9027391629793018
0.9584999735602959	0.1290222602086830	0.0939971278679261
0.9728309831436591	0.1375899847775799	0.5694636954041282

0.9454736636986186	0.2676352832154077	0.4250797107387241
0.1919444509189674	0.1938900350017889	0.7628300795953340
0.1968365666470807	0.2024346244961873	0.2370481519884800
0.9442467214803069	0.2702450489343677	0.9051713628401576
0.1537599158708780	0.3326845529741329	0.0945206380033700
0.1668544297336521	0.3347805830457876	0.5739769420950436
0.1339093480442829	0.4638413146070448	0.4287837188674589
0.3915875367802766	0.3978448017491930	0.7638069498047345
0.3783362991443039	0.3931236948502662	0.2401585849209150
0.1277973615758086	0.4690857668623221	0.9064955196317998
0.3612394506854723	0.5283878524763748	0.0970513068412030
0.3661405386600481	0.5353618200985765	0.5690093225371594
0.3355278498118273	0.6700362601158013	0.4243543817111958
0.6065267228177043	0.5983150945176168	0.7633282935367106
0.5985827013149104	0.6036177580161955	0.2366218010349706
0.3166921660876770	0.6665141382716727	0.9076950682939594
0.5595581082691383	0.7333805143451975	0.0938024940574839
0.5656784055251914	0.7350766368889374	0.5709962856583561
0.5370310771390175	0.8659165428865367	0.4280261288357623
0.8139984210661032	0.8011262632001959	0.7584023371413104
0.7834725237265477	0.7927375841882243	0.2399512988953944
0.5319198492491295	0.8658680647639450	0.9046351603977107
0.7716965559633248	0.9318068141857833	0.0902577240523397
0.7781452612102209	0.9365874818774915	0.5685536231877799
0.2229399537166835	0.0611270042070059	0.4260970315427439
0.5032555162966478	-0.0040485083317099	0.7621688854000944
0.5094065434152406	0.0015703156236615	0.2361594911237662
0.2290200027605706	0.0668072851839650	0.9053934736264974
0.4759992510221605	0.1347694717380274	0.0949271675135842
0.4511737533667797	0.1313089496630536	0.5714731994114497
0.4273505082523290	0.2624175716219590	0.4291509770466360
0.7099424223842085	0.1986452902274154	0.7622340742599163
0.7113574612359295	0.2049172613646596	0.2395051181693203
0.4287392298156353	0.2674551890914449	0.9044700606719437
0.6670878728524886	0.3308712070912557	0.0975912414773050
0.6626761551821603	0.3358656723015305	0.5695798191930510
0.6380416784911525	0.4673475041805959	0.4240739458346835
0.9035042618346228	0.3978689251561632	0.7633311144845683
0.9045726101180989	0.4055058438105070	0.2376169265042189
0.6208962708693222	0.4654092765880855	0.9109031727093461
0.8838638296033158	0.5412822024901884	0.0930777144348166
0.8607033312676007	0.5290488073311761	0.5754507655151290
0.8373477569893728	0.6654828107650410	0.4283069039095608
0.1112660743478598	0.6034448113190251	0.7574972711270416

0.1039381743653379	0.6003201237569540	0.2394034800916949
0.8384664257758280	0.6636143359180232	0.9093469698947760
0.0668230599549390	0.7297916357506485	0.0965854403379567
0.0646707034944564	0.7365335988187945	0.5693327904147877
0.0323039639620402	0.8629007769360960	0.4248438166861911
0.2980003491753068	0.8008033683082985	0.7589405278672514
0.2935816301295296	0.8010825680101774	0.2422581327284138
0.0310992884211889	0.8666561710577078	0.9047619172012764
0.2836233140755642	0.9355674675701513	0.0877361100222376
0.2557750608013548	0.9327154819634129	0.5706986360250176
0.4317170210131319	0.2693380399736893	0.1694609704564011
0.2670256730076264	0.9315279084161149	0.8323801540936667
0.3004004752848341	0.7994991381797926	0.4960586562141788
0.6663938483165733	0.3337539270834261	0.8346783676761005
0.9010890784113275	0.4007219182484387	0.5004225002201399
0.8328868152757243	0.6675022379586283	0.1653496796268157
0.9691011314459629	0.1323429150541912	0.8331445582840282
0.7369572017131837	0.0659797073690713	0.1658674211758429
-0.0000926830011788	0.0000101306738269	0.4972948564461168
0.1648492760984400	0.3326342414773940	0.8340820808511327
0.9314947497256331	0.2672033573367592	0.1668351646551242
0.1999041090355041	0.1989190553586994	0.4985856069457681
0.3595282886006007	0.5343545485952736	0.8347604581310680
0.1302183303130862	0.4663003996727031	0.1671201415496406
0.3978090452894180	0.3995651858425971	0.4994117361812793
0.5710734966236405	0.7321132651475796	0.8343459693568714
0.3311342265410027	0.6669737311649426	0.1676005119667278
0.6019061457781475	0.6005142621043359	0.4981712398586648
0.7692636638210325	0.9330606859501702	0.8326963545750179
0.5322792312182902	0.8674331039506977	0.1653729786031200
0.8022351964111386	0.8006181579813760	0.4979165197670872
0.4664020382634871	0.1328026601517627	0.8331749672300933
0.2298005348877143	0.0653023904204460	0.1657780789838860
0.4977946221722647	0.0007096121260889	0.4981382181482865
0.7014202385842268	0.1994323983520610	0.4986822653972772
0.8698920394754917	0.5337098683360804	0.8349844477937758
0.6340742122128440	0.4672399444581338	0.1669836998035621
0.0646840471630006	0.7335362781947751	0.8328783937021040
0.0997083854516944	0.5998041740199865	0.4989072701578967
0.0337736948012229	0.8676353064573944	0.1662119647309238

$E_0 = -620.80505 \text{ eV}$

(811)

1.000000000000000

6.0972377343993216 0.6558740360166482 0.0547047560884840

0.0385779159282136 12.1972817578942045 -0.4905801289277218

0.1926347257700361 -0.5420079283565232 14.3028488328156571

Li O Mn Co Ni

30 60 3 3 24

Direct

0.9659644751522117	0.1351414166667373	0.3324116348765430
0.7343327719507811	0.0679359928765005	0.6606700503379971
-0.0015579751780034	0.0016641756777569	0.0033413994982653
0.1603029489454545	0.3319212417555378	0.3328188763861097
0.9338417693608911	0.2660585889102456	0.6592020870213965
0.1927222746151374	0.1998957375468648	0.0033038909703444
0.3639575295273293	0.5339643035757430	0.3314400214271411
0.1300552161686267	0.4696974188606189	0.6586397546520896
0.3993890043346245	0.4003916171729471	0.0055620554163760
0.5711433552038085	0.7363379899622746	0.3300960233095599
0.3306319077489210	0.6689686319161215	0.6600184231829598
0.5985585084446488	0.6016156060106641	0.0020538831256558
0.7685375532554021	0.9306468053744961	0.3362872295263011
0.5437603895712333	0.8666188775988333	0.6579086499544291
0.7985613932252408	0.7980790896682136	0.0057698475078378
0.4645532841284004	0.1336437208313095	0.3336187576528331
0.2303514004296262	0.0691902832013459	0.6597203341112869
0.5019447331102130	0.0012072091316300	0.0046847532757712
0.6753139397262560	0.3327676953877275	0.3337159905122957
0.4379176689914528	0.2633037292820981	0.6630581103072983
0.7077505812660022	0.1997068684507534	0.0032039366933182
0.8702371500018614	0.5359053509309636	0.3333082387017864
0.6339403278706374	0.4676796072696292	0.6598192818333881
0.9006129933086796	0.3979965336692781	0.0048693114986365
0.0586011776932220	0.7341962002680446	0.3334248413829273
0.8344163683393153	0.6686912256266369	0.6587720100297053
0.0998973809662823	0.6013305830971760	0.0028304677480576
0.2690913937960033	0.9300217558369200	0.3361450958952160
0.0212930536720451	0.8684864109667491	0.6581862111790693
0.3006059306847587	0.7978032794747497	0.0060776820706512
0.7283122043369352	0.0671015017773343	0.4241418219091784
-0.0082896758486193	-0.0052182291202514	0.7628643165828595
-0.0091939752458245	0.0010941676090020	0.2400447430746922
0.7255683680116723	0.0687353056389211	0.9063042360715003
0.9548074350174836	0.1318202833461494	0.0925503291978007
0.9685659809048793	0.1351675583946097	0.5701685242225969

0.9145168841414490	0.2651797639010958	0.4203687259852752
0.2080050124860387	0.1965244769137687	0.7620371974656713
0.2093524320175591	0.2001502382868207	0.2380567816933518
0.9282150568777888	0.2707895091259709	0.9010961914452374
0.1725870921608204	0.3323897706864450	0.0934730593092404
0.1508518250142477	0.3343899584219366	0.5680600310899980
0.1144006159341818	0.4671894714019424	0.4242674401095448
0.4044987502055390	0.3957843243243796	0.7640931450598418
0.4118730580419201	0.4019423885146007	0.2384985256684304
0.1260677705344049	0.4678495840788383	0.9062528269501688
0.3711795844307100	0.5325282084808739	0.0979534189189113
0.3728199071359541	0.5332259094589973	0.5692318460957707
0.3318232777815748	0.6690851020505649	0.4232361737072509
0.6107266152613346	0.5972560510135251	0.7615526192506916
0.6165035529696387	0.6018527562006514	0.2387940703018916
0.3498468227631711	0.6690998738212317	0.9071648934426491
0.5872593051420554	0.7332720242045704	0.0955043575234005
0.5567415003899348	0.7342769243360032	0.5708101893632710
0.5292787111334130	0.8668283200574949	0.4253914434560567
0.7812043859053883	0.7987319521740406	0.7593121770551325
0.8110283231875195	0.8027086513369123	0.2427566492648240
0.5388109466885722	0.8694912559139638	0.9046555396811872
0.7662223423508243	0.9332886221274809	0.0934677717781604
0.7553874136749674	0.9340366512534800	0.5724336193142988
0.2490756502928220	0.0661407934462191	0.4275021930571845
0.5071250669753284	-0.0050396029615488	0.7640478685461923
0.5088845708673698	0.0017328699449193	0.2370328358860745
0.2413425599383864	0.0640608026556986	0.9055652683229802
0.4735551217222129	0.1346305788411526	0.0932835617189036
0.4859952414028814	0.1331560280216072	0.5743540243744465
0.4356674416109175	0.2651872689331018	0.4266922605394619
0.6869219948084336	0.1978851963426946	0.7584910294443392
0.6952091890533575	0.2014799519280652	0.2383011371461364
0.4364549287639711	0.2703555417383222	0.9033474122170961
0.6590345507550484	0.3330058081072041	0.0931361646979740
0.6872936987837145	0.3333920453751160	0.5723494788362053
0.6514000424935174	0.4626905034233927	0.4272348745423683
0.8998040173825105	0.3959102228340732	0.7638118434359417
0.8942279579170356	0.4014660045759516	0.2352697476047893
0.6352211096818152	0.4717741205029451	0.9044606763486717
0.8521131764872565	0.5305511113909711	0.0921279442580649
0.8649460991243235	0.5337010619739802	0.5763595062815577
0.8299043551566369	0.6665484191726391	0.4268484336307729
0.0987871299909652	0.5959512404841766	0.7638531951006023

0.0788382884544169	0.6011664493434765	0.2384809597906750
0.8367097426974029	0.6666970046051246	0.9061593567325394
0.0540411036161369	0.7318896496339377	0.0942446263548420
0.0721217404420494	0.7320855691537664	0.5723921747739147
0.0385727165786488	0.8653286951894165	0.4265643761011673
0.2950633846377049	0.7991716892440119	0.7652765770405396
0.3030665321471535	0.8021084234075254	0.2398993629752460
0.0192257310604056	0.8704139532927263	0.9035622361745285
0.2524204123403795	0.9313122880715531	0.0937773951205789
0.2712717441215956	0.9299639106046402	0.5722391807751954
0.4351807650773162	0.2668805812303804	0.1670494061035399
0.2645974830542567	0.9339246107265354	0.8343584781318851
0.2995482292506281	0.7980739672781182	0.4972185048233767
0.6656296742786116	0.3334799355755095	0.8328013766846236
0.9001167847299730	0.3988771478294750	0.4979612842467682
0.8338243834981141	0.6660070107173218	0.1669356495669192
0.9618310504479466	0.1339882028117947	0.8318411620766482
0.7335837171498042	0.0675425105903986	0.1676473998013703
0.0003516290524257	0.0012444691857002	0.4970898778307277
0.1671242836831743	0.3328875306934826	0.8331733493746747
0.9326089895207615	0.2651848324549348	0.1660622632742246
0.2003670230605480	0.2012737238500369	0.4974669690806338
0.3708927271926744	0.5340473632743924	0.8345808629971652
0.1297871700294091	0.4681653773301029	0.1664424409614876
0.4002416386017464	0.3996688206766455	0.4977177104881280
0.5708770315555646	0.7319447252096570	0.8334031413557718
0.3350790961773669	0.6662496226880433	0.1676874867959031
0.6065337830550074	0.5980259440649273	0.4995435264678786
0.7614585693698590	0.9331751166515574	0.8337523891676775
0.5381069470533751	0.8671083282449595	0.1672916172553685
0.7973890190307863	0.7995192686924298	0.4982516298433262
0.4690680523609344	0.1341903628943101	0.8338175104463359
0.2330880229245187	0.0645802649526696	0.1678109740292320
0.5056952856462608	0.0021433583219453	0.4980943385228581
0.7031647559519989	0.2011370002862913	0.4972470907811141
0.8671412221394896	0.5329438726330821	0.8342214064051485
0.6390922528177289	0.4678415833322889	0.1666120875602390
0.0619413371943889	0.7321638351600793	0.8343613589379281
0.0965135985298640	0.5985310673131293	0.4988061868870227
0.0291701485444695	0.8670416433230782	0.1679853031988759

$E_0 = -593.72768 \text{ eV}$

(71515)

1.000000000000000

5.7613873212826165	0.6949479265884444	-0.0189555724162684
0.0700373631033306	12.5975652378108176	-0.0315980270212684
-0.0429951200483291	-0.0358866816187024	14.2932797763206256

Li	O	Mn	Co	Ni
30	60	4	5	21

Direct

0.9617305173090515	0.1324087522199443	0.3322072654460887
0.7320309895379041	0.0648871904143962	0.6648465660908296
0.0001594717370480	0.0019805616146174	0.0003872733544394
0.1623768448865226	0.3361610690013507	0.3323414915571283
0.9344800601246207	0.2666882765985554	0.6656770984733595
0.2006540076767268	0.1983987230836748	0.0011504598960817
0.3671110997955772	0.5334624664475598	0.3326482734927240
0.1343484503734193	0.4681556616718492	0.6659104857969904
0.4017529452104947	0.3976108014537593	0.9995426634304625
0.5701556005860267	0.7303429127328245	0.3330574094250844
0.3312601492730125	0.6686360116765231	0.6672799964749713
0.6038607172655651	0.6012827434746548	0.9982405350787974
0.7681659541366025	0.9346909325280104	0.3333185870488968
0.5303851997649214	0.8671972303767275	0.6656380893995215
0.7984270986081076	0.8000075095565573	0.9990146947394158
0.4702114553934514	0.1324654779344058	0.3329662373072010
0.2370851498240022	0.0650952454986122	0.6658759388270359
0.5002185853502177	-0.0005391167172777	0.0020355837001102
0.6677307391488786	0.3334751365492418	0.3335095360924776
0.4288867596545992	0.2656708030833664	0.6664885055052073
0.6977619410810232	0.2009824740288936	0.9989187538125762
0.8664383606838454	0.5329093242899998	0.3321188224735779
0.6343301995605105	0.4681139884555900	0.6664152810592099
0.9006594673510824	0.3987359665754311	1.0002433688240824
0.0676336850128871	0.7329236804132944	0.3315351065967161
0.8360709191760891	0.6678117803410850	0.6679205056708781
0.0973710699119522	0.6008274273325291	0.9986783944877912
0.2624022624303566	0.9343829093388791	0.3327584598419353
0.0377905427422947	0.8637773216398005	0.6656075765898378
0.3043362187883408	0.8012786203728064	0.9971816976768504
0.7414094919804820	0.0701668889713687	0.4231371724495162
0.0132188195106405	1.0058173012406035	0.7585607208431214
0.9880359653748890	0.9962273240679265	0.2429399759444792
0.7550836124834436	0.0720737545834785	0.9058558539788751
0.9679621033412020	0.1248299073360750	0.0951474078916898
0.9549932532975451	0.1291064812518127	0.5717078253266854

0.9427449417588593	0.2726216682858201	0.4242503505054828
0.1801614057305389	0.1972665496789378	0.7597299648145954
0.2168011893027723	0.1968241163720917	0.2404748740650264
0.9212486697477702	0.2626988828794041	0.9084709501874880
0.1832709700358087	0.3303965755278724	0.0876756120524991
0.1566045994556170	0.3389155051892733	0.5771330210063103
0.1271042500407226	0.4594428383680484	0.4245576969597252
0.4140645989155866	0.3929370361274998	0.7531805782345682
0.4011845826751733	0.3925773708271615	0.2441031306636674
0.1199926081407826	0.4710419267962220	0.9063852831033623
0.3532443037978109	0.5371002549030532	0.0947746610513668
0.3837206594322324	0.5298639902369442	0.5696874494305910
0.3316558591467209	0.6725202993938504	0.4204699769887153
0.6099135509741049	0.5948727774588352	0.7579021507868816
0.6084037781852490	0.6062111237663840	0.2407784105203989
0.3219794713568703	0.6718846366776845	0.9081447324110590
0.5733949442024163	0.7284627315178296	0.0902314136768868
0.5489192747058966	0.7348522571083707	0.5763949377648390
0.5168477959701823	0.8676522473356784	0.4237672060021964
0.8146976224826661	0.7952252813662299	0.7584114441845028
0.7881901731623586	0.7930112384101354	0.2407124834361145
0.5226219834236050	0.8738270548551638	0.9122555724198826
0.7736522694268156	0.9368118698809648	0.0933023747069490
0.7667287751053775	0.9404904907014263	0.5703251079079815
0.2255541655416073	0.0608667189180172	0.4268909424257539
0.4918930630660318	0.9962925079004804	0.7561404614009292
0.5063423330488930	0.0054837144661008	0.2388394327345409
0.2199714921967413	0.0660614491622902	0.9072992679895943
0.4832208947145201	0.1365490296126116	0.0896529217494157
0.4592866210518037	0.1307809320819886	0.5781768840961888
0.4466778904088896	0.2678467000530217	0.4288566537259711
0.7153146619452989	0.2029129761256741	0.7582051005164927
0.6932412194563932	0.1974108662217283	0.2410863446749829
0.4410297782159420	0.2708405804165782	0.9078141003721341
0.6570052668736506	0.3299208712644720	0.0895269073005297
0.6855930757635351	0.3331048441632639	0.5711626301327440
0.6510547117833285	0.4621577523257114	0.4232490134129038
0.8838369610005817	0.4012061124270820	0.7597547967340434
0.9121207194437463	0.4042594256704569	0.2400203602623478
0.6283745262940095	0.4590441838207668	0.9111572200455095
0.8644537794958902	0.5433737049718533	0.0921281680209280
0.8685727859474477	0.5232307943595950	0.5741250673762969
0.8186320059814414	0.6625372265023917	0.4258118894498204
0.1040650112683990	0.6033504558101654	0.7528619788913282

0.0826119718819121	0.6057262393600883	0.2415436864297928
0.8328833860928866	0.6616891273861223	0.9092720448853628
0.0446388787021702	0.7345206133336364	0.0935123018367679
0.0774389242645324	0.7368567161722978	0.5759090657097740
0.0391592781298941	0.8685761083227239	0.4239137472205583
0.3047334204029324	0.8086227482324023	0.7563284483841177
0.2858582317065059	0.7983411859222262	0.2374420260022387
0.0503321833856482	0.8666525942268701	0.9077716636247530
0.2733500204583109	0.9380282538687400	0.0908924521491285
0.2508506839941962	0.9291544894678135	0.5734381476478453
0.4380924884620275	0.2664485341226173	0.1649788725001775
0.2727208433583851	0.9329095874053319	0.8330329177895279
0.2956337901413271	0.7990757306780031	0.4991460434939153
0.6607323254176610	0.3348759016322793	0.8333666251451342
0.9061082378126586	0.3992940534264152	0.4987008924538443
0.8263874521758305	0.6669802473335174	0.1666399482505766
0.9673086022264976	0.1342125397584350	0.8329670886622385
0.7355868284252340	0.0656642819367056	0.1668150916532488
0.9968461771242274	0.0003834906443352	0.4982622990039145
0.1631923453156071	0.3343296893060841	0.8328395269896615
0.9365857146528580	0.2664913633705155	0.1656877563090121
0.1994399589616128	0.2006574990871046	0.5013808509056216
0.3648460299446507	0.5335606627712964	0.8317861805078459
0.1324246704918659	0.4680980928976343	0.1666855682612907
0.4055890424571728	0.3988947727789251	0.4992256863643847
0.5690492977580144	0.7332290396411502	0.8334941639381920
0.3271768081848614	0.6678425444965592	0.1660944268222806
0.6021634785744160	0.5981888180035627	0.4985172513828678
0.7710960079266976	0.9331715198462509	0.8328557044442532
0.5318916888833058	0.8660091361378904	0.1653333174204641
0.7966756325331567	0.7994429949355104	0.4996902659983610
0.4678895283884756	0.1335623308577723	0.8324802703850660
0.2363040996904294	0.0650393287677947	0.1670294449642677
0.4960306301824682	0.0015040220855844	0.4992033523851942
0.7023082041810270	0.1989323087690684	0.4999590567033999
0.8653069045518398	0.5347071131191599	0.8322588348499065
0.6336624611440302	0.4674872081922216	0.1666661054879948
0.0690771210106749	0.7317632346570886	0.8325834109018611
0.0996430104532658	0.5989228687559001	0.4990154744958533
0.0284546914933018	0.8673698989143727	0.1659368488410944

$E_0 = -590.81245 \text{ eV}$

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1. (a) Blöchl, P. E., Projector augmented-wave method. *Phys. Rev. B* **1994**, *50*, 17953-17979; (b) Kresse, G.; Joubert, D., From ultrasoft pseudopotentials to the projector augmented-wave method. *Phys. Rev. B* **1999**, *59*, 1758-1775.
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3. Perdew, J. P.; Burke, K.; Ernzerhof, M., Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1996**, *77*, 3865-3868.
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