Accurate Band Gap Predictions of Semiconductors in the Framework of the Similarity Transformed Equation of Motion Coupled Cluster Theory

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I. Geometric structures of the semiconductor study set

1. Oligoacenes and oligothiophenes

Naphtalene (2A), Anthracene (3A), Tetracene (4A) and the Pentacene (5A) are four members of oligoacene molecules. In general oligoacene molecules can be thought as aromatic derivative molecules of benzene. They are rigid and planar and this planarity is preserved in the crystalline environment. At ambient conditions 2A and 3A crystallize in monoclinic space group $P2_1/\alpha$ while 4A and 5A crystalize in triclinic space group $P\bar{1}$.[1] Similarly α-2T, α-3T, α-4T, α-5T, α-6T oligothiophenes are five members of oligothiophene molecules that are thiophene and crystalize in monoclinic space group $P2_1/\alpha$ or $P2_1/c$ space groups.[2]

2. Alkali metal halides

The first class of the considered inorganic semiconductors are the alkali metal halides (LiF, NaF, LiCl, NaCl, KCl, LiBr, NaBr, KBr). All of them crystalize in the rock salt structure (Fm-3m space group) with cubic unit cells $[X_4Y_4]^0$ and octahedral (O_h) non-distorted building blocks $[XY_6]^{5-}$.[3-5] Table. S1 shows all distances of the highly ionic bonds X-Y.

3. Metal-Oxides, Metal-Sulfides, Metal-Selenides

The second class of inorganic semiconductors is constructed from a variety of metal oxide and metalsulfide and metal selinide solids as shown in Table S1. Besides the rock salt structure the other most often occurring structure is the zinc blende. Its basic building blocks $[ZnS_4]^{6-}$ are all tetrahedral (T_d).[3-5] In general these

semiconductors show bonds that are more covalent (smaller bond lengths) than the semiconductor list of alkali metal halides while.

II. Figures

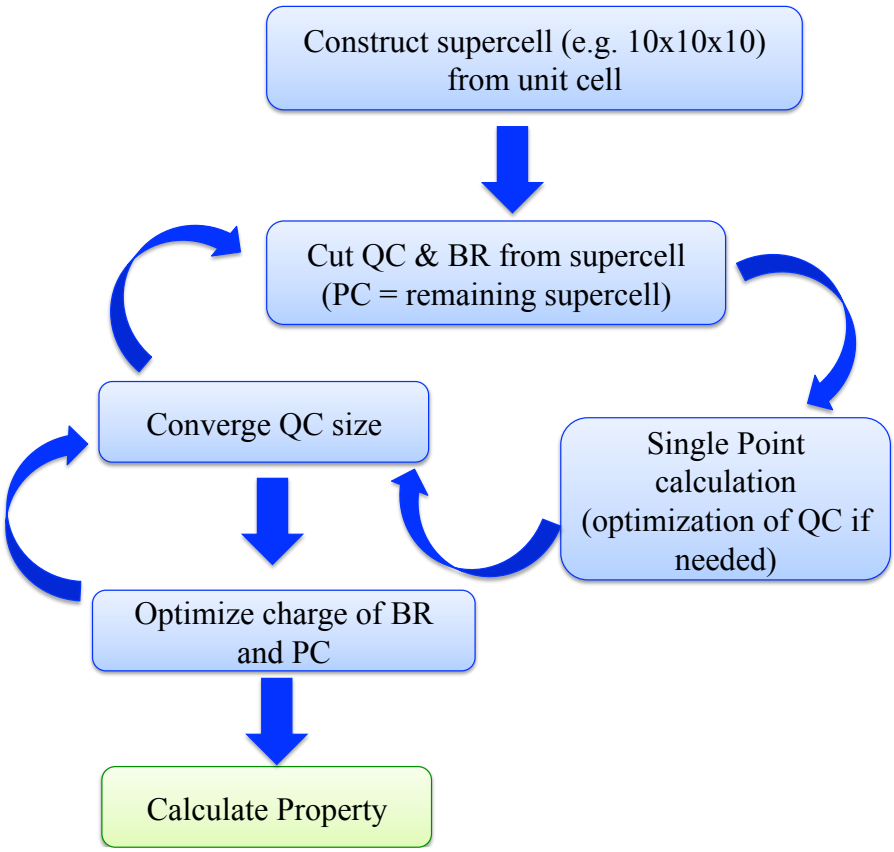

Figure S1.
Computational protocol for the calculation of properties with the embedding approach.

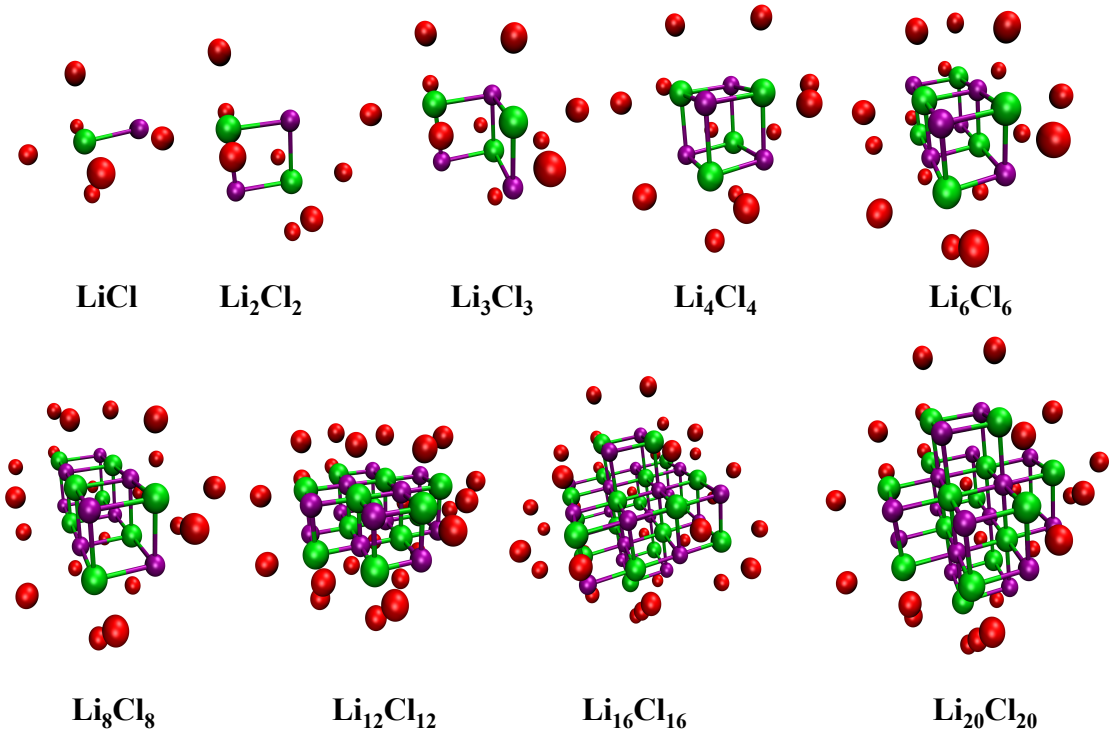

Figure S2.
Graphical representation of system growth (QC+BR) of LiCl (Unit Cell/Neutral Approach). Representative for all rock salt structures. Colour coding QC: Li (purple), Cl (green), BR: cECPs (red).

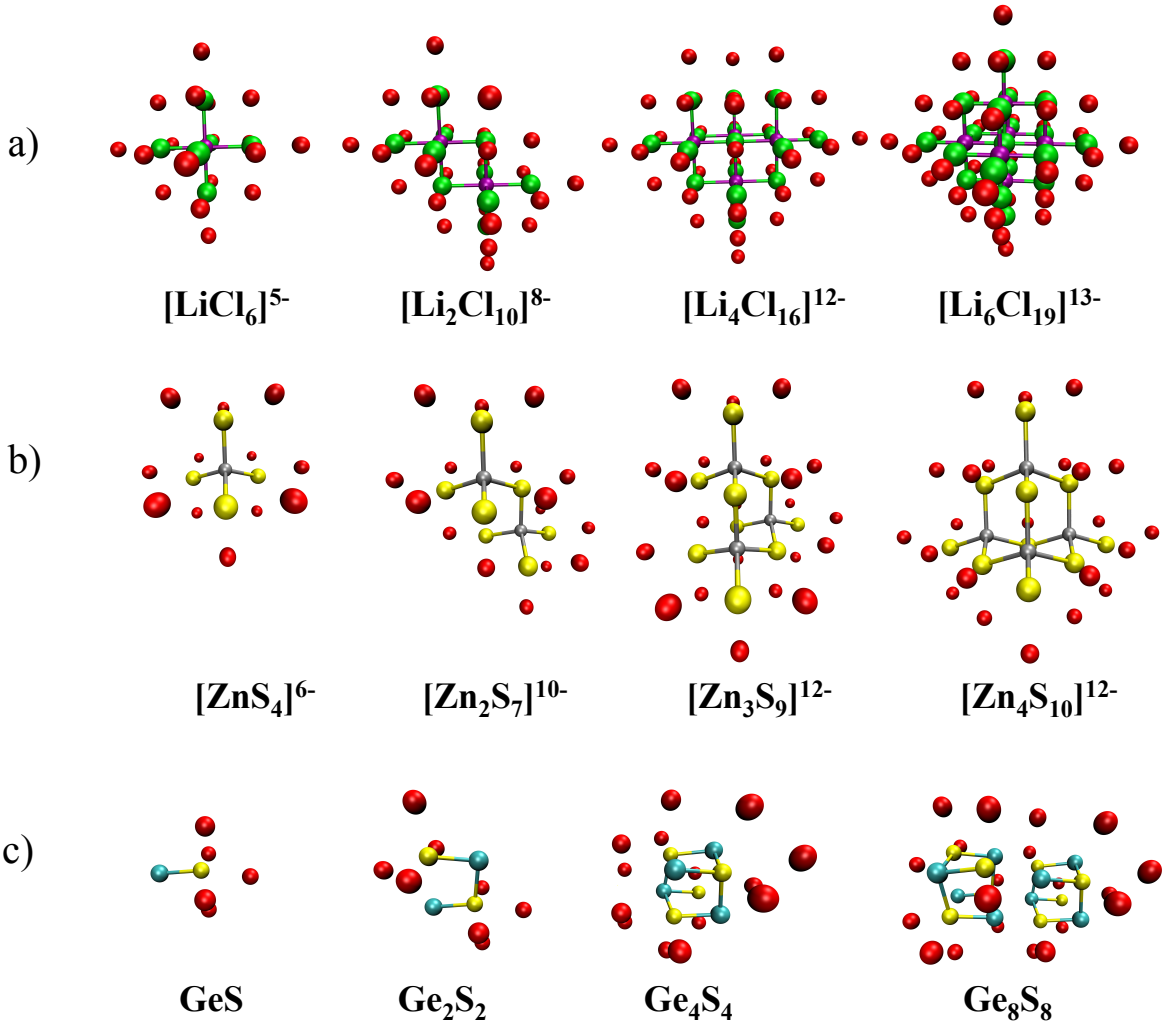

Figure S3.
System growth (QC+BR) of a) LiCl (Ligand Field Approach). Representative for all rock salt structures b) ZnS (Ligand Field Approach). Representative for all zinc blende structures and c) GeS (Unit Cell/Neutral Approach). Representative for all orthorhombic structures. Colour coding QC: Li (purple), Cl (green), Zn (grey), Ge (cyan) BR: cECPs (red).

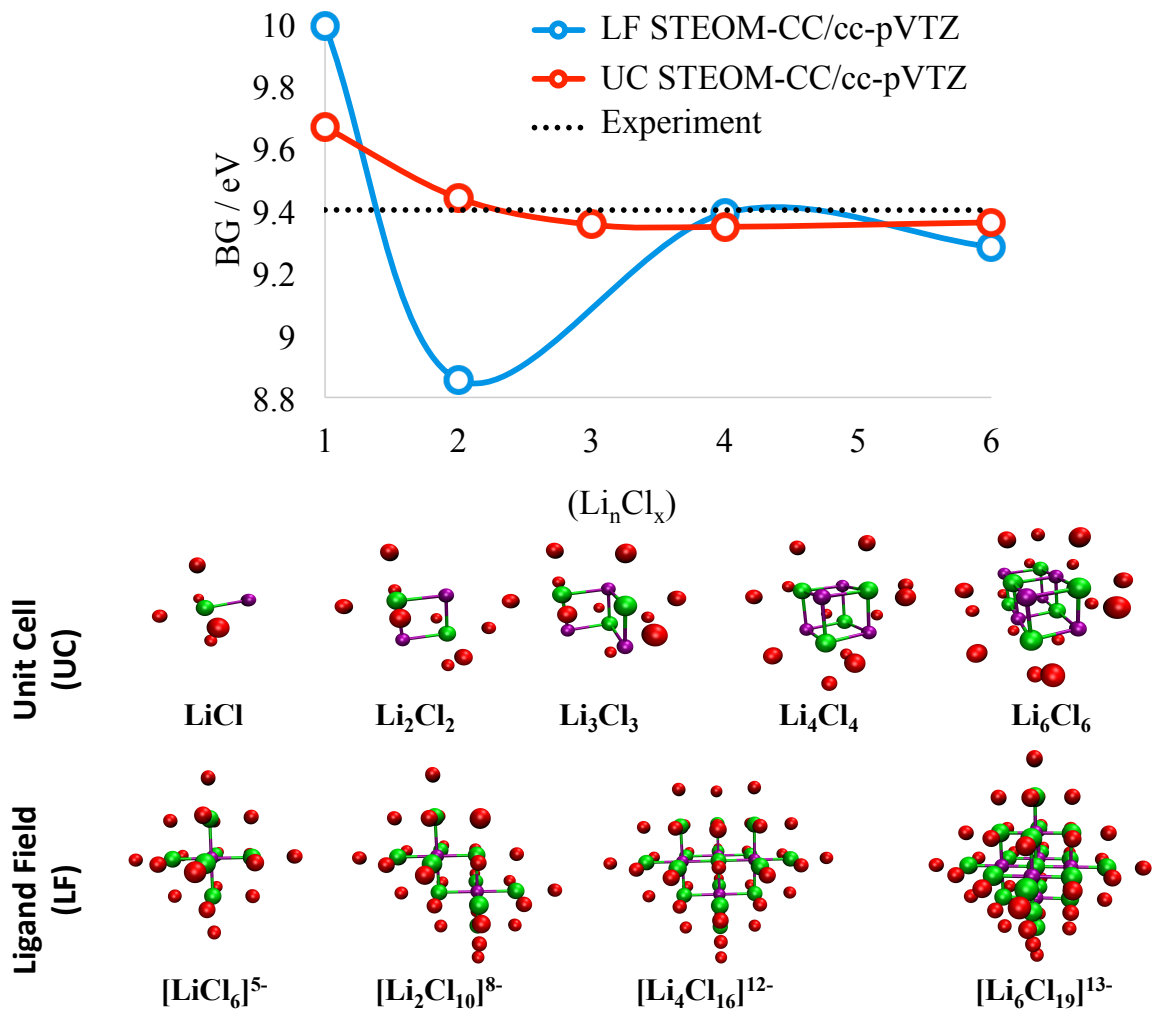

Figure S4.
LiCl system growing (Li_nCl_x, n=1-6) and cluster size convergence at the STEOM-CC/cc-pVTZ level by employing the Unit Cell (UC) and the Ligand Field (LF) approaches

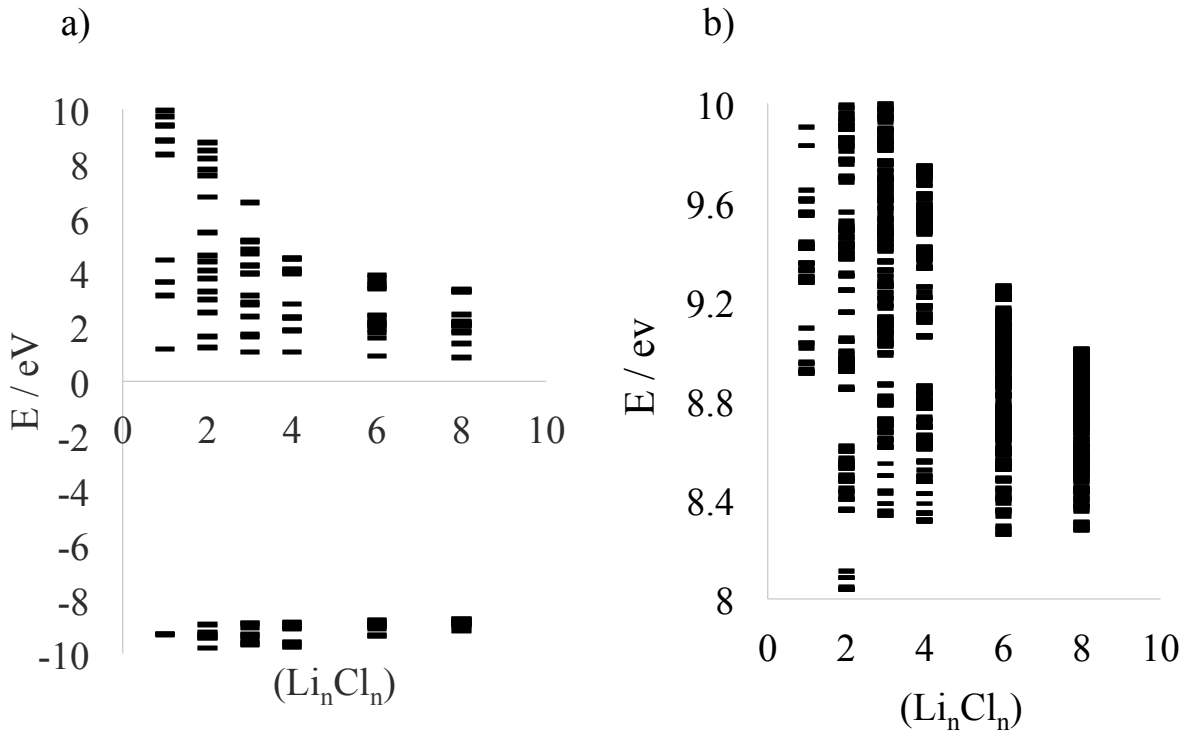

Figure S5.
B3PW91/cc-pVTZ TD-DFT calculated a) MO energies around the HOMO-LUMO gap and b) excited state energies as a function of growing cluster size of LiCl.

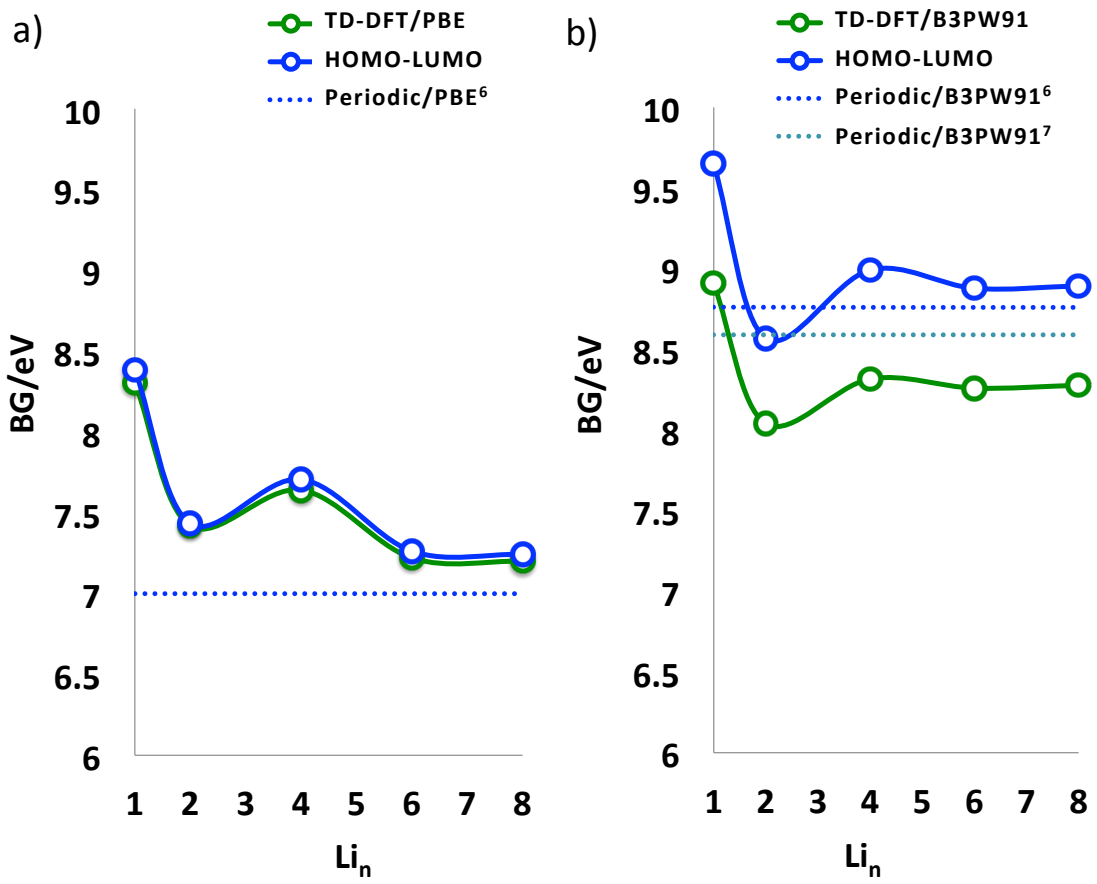

Figure S6.
Experimental versus DFT and TD-DFT calculated band gap energies for clusters $[Li_nCl_n]^0$, n=1-4, 6 and 8 by employing a) PBE and b) B3PW91 functionals. Color coding DFT/PBE or B3PW91 (solid blue line), TD-DFT/PBE or B3PW91 (solid green line) and Periodic DFT/PBE or B3PW91 (dotted blue[6] or cyan line[7]).

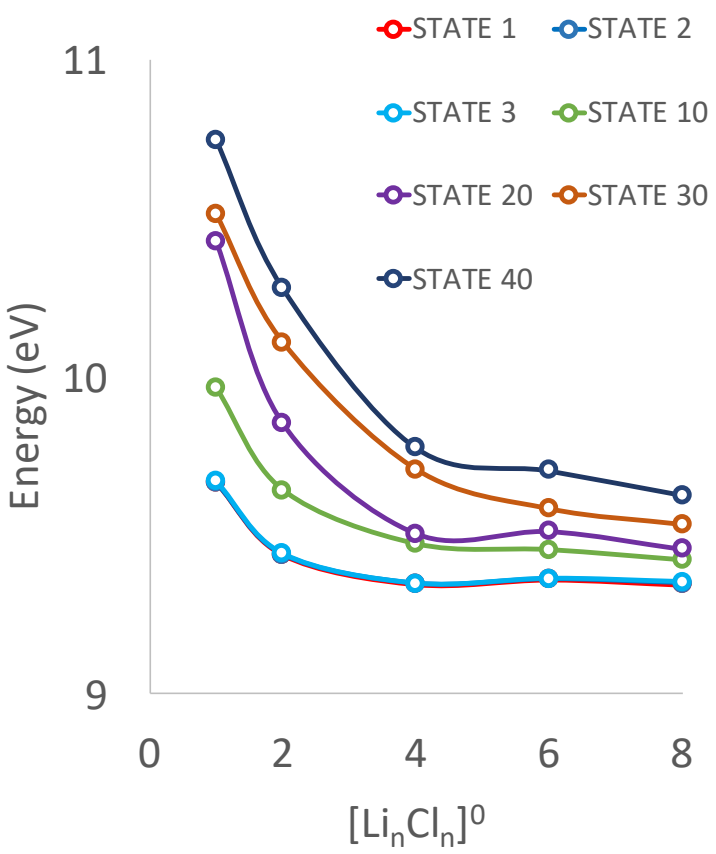

Figure S7.
bt-PNO-STEOM calculated excitations energies for clusters $[Li_nCl_n]^0$, n=1-4, 6 and 8. Red, blue, cyan, green, purple, orange and dark blue lines represent excitations states with numbers 1, 2, 3, 10, 20, 30 and 40 respectively.

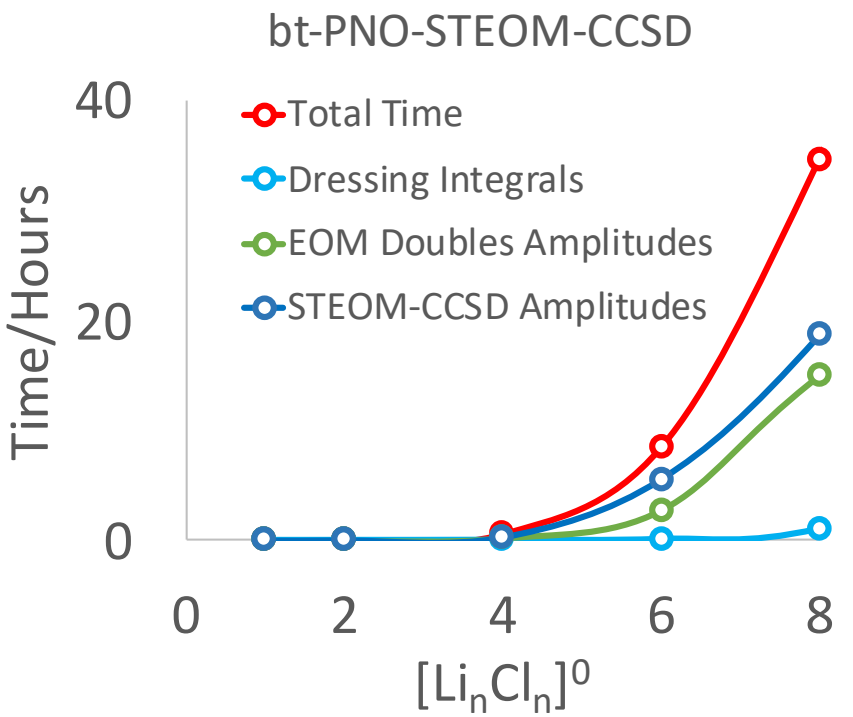

Figure S8.
Scaling of the bt-PNO-STEOM-CCSD calculations as a function of the increasing cluster size in the calculations of the energy band gaps of $[Li_nCl_n]^0$, n=1-4, 6 and 8 clusters. The times are analyzed in terms of Total time (red line) as well as individual timinngs spent in computing the Dressing integrals (cyan line) and in solving the STEOM-CCSD (blue line) and the EOM doubles amplitudes (green line). The calculations refer to parallel runs with 4 processors.

III. Tables

Table S1.
Crystallographic data and experimental energy gaps for olicoacene and α -olithiophene organic semiconductors

Molecule	Crystal Structure	Optical band gaps (eV)	Fundamental band gaps (eV)
		Oligoacenes[1, 8-9]	
2A	$P2_1/\alpha$	4.14	8.19
3A	$P2_1/\alpha$	3.20	6.87
4A	$P\bar{1}$	2.54	5.51
5A	$P\bar{1}$	1.84	4.80
		α -Oligothiophenes[10]	
α-2T	$P2_1/\alpha$ or $P2_1/c$	4.11	7.70
α-3T	$P2_1/\alpha$ or $P2_1/c$	3.49	6.44
α-4T	$P2_1/\alpha$ or $P2_1/c$	3.18	5.76
α-5T	$P2_1/\alpha$ or $P2_1/c$	2.98	5.40
α-6T	$P2_1/\alpha$ or $P2_1/c$	2.87	5.20

Table S2.
Crystallographic data and experimental energy gaps for study set of inorganic semiconductors

Solid	Bond length X-Y / Å	Space Group	Range of Experimental Band Gaps (eV)	Energy band gaps (eV) based on Optical Absorption Experiments
LiF	2.022	Rock Salt (Fm-3m)	11.60-14.20[11-16]	11.60[16]
LiCl	2.586	Rock Salt (Fm-3m)	9.40[15, 17]	9.40[15]
NaCl	2.820	Rock Salt (Fm-3m)	8.50-9.00[18-22]	8.97[20]
LiBr	2.745	Rock Salt (Fm-3m)	7.60[19]	7.60[19]
NaBr	2.954	Rock Salt (Fm-3m)	7.00-7.50[18-19, 23]	7.50[19]
MgO	2.109	Rock Salt (Fm-3m)	5.40-7.90[24-28]	6.21[28]
MgS	2.830	Zinc Blende (F-43m)	4.50-5.50[29-31]	4.78[30]
MgSe(ZB)	2.937	Zinc Blende (F-43m)	3.59-4.10[32-38]	3.81[37]
MgSe(RS)	2.073	Rock Salt (Fm-3m)	3.90[35]	3.90[35]
ZnS	2.673	Zinc Blende (F-43m)	3.66-3.78[34, 39-40]	3.78[39]
ZnO	2.315	Zinc Blende (F-43m)	3.10-3.44[41]	3.44[41]
ZnSe	2.871	Zinc Blende (F-43m)	2.68-2.82[33, 42-44]	2.82[43]
GeS	1.820/2.150	Orthorhombic (D^{16}_{2h})	1.54-1.74[45-47]	1.55[47]

Table S3.
Sizes of Quantum Clusters with optimized charges to equip the BR and PC regions that were employed to represent the solid structure of the studied inorganic semiconductors. The minimum cluster unit that required to show convergence of the computed band gap energies in the TD-DFT and bt-PNO-STEOM-CC calculation is also presented.

Solid	Space Group	Largest Cluster size tested	Converged Cluster size	Charge of cECP and PC
LiF	Rock Salt (Fm-3m)	$Li_{20}F_{20}$	Li_6F_6	±1.23
LiCl	Rock Salt (Fm-3m)	$Li_{62}Cl_{62}$	Li_6Cl_6	±0.95
NaCl	Rock Salt (Fm-3m)	$Na_{20}Cl_{20}$	Na_6Cl_6	±0.93
LiBr	Rock Salt (Fm-3m)	$Li_{12}Br_{12}$	Li_6Br_6	±0.79
NaBr	Rock Salt (Fm-3m)	$Na_{12}Br_{12}$	Na_6Br_6	±0.86
MgO	Rock Salt (Fm-3m)	$Mg_{20}O_{20}$	Mg_6O_6	±1.70
MgS	Zinc Blende (F-43m)	$[Mg_8S_{19}]^{22-}$	$[Mg_4S_{10}]^{12-}$	±0.80
MgSe	Zinc Blende (F-43m)	$[Mg_8Se_{19}]^{22-}$	$[Mg_4Se_{10}]^{12-}$	±0.68
	Rock Salt (Fm-3m)	$Mg_{12}Se_{12}$	Mg_6Se_6	±1.51
ZnS	Zinc Blende (F-43m)	$[Zn_8S_{19}]^{22-}$	$[Zn_4S_{10}]^{12-}$	±0.47
ZnO	Zinc Blende (F-43m)	$[Zn_8O_{19}]^{22-}$	$[Zn_4O_{10}]^{12-}$	±0.76
ZnSe	Zinc Blende (F-43m)	$[Zn_8Se_{19}]^{22-}$	$[Zn_4Se_{10}]^{12-}$	±0.39
GeS	Orthorhombic (D^{16}_{2h})	$[Zn_8S_{19}]^{22-}$	$[Zn_4S_{10}]^{12-}$	±0.47

Table S4.

TD-DFT and bt-PNO-STEOM-CC/CBS calculated optical band gaps ($\Delta E_{O}^{S_0 \rightarrow S_1}$, eV). Statistical evaluation of all quantities is given by means of mean absolute error (MAE) and maximum absolute errors (MaxAE).

	BP86	BLYP	PBE	B1LYP	B3LYP	B3PW91	PBE0	B2PLYP	STEOM-CC	Experiment
Organic Semiconductors										
2A	4.26	4.26	4.26	4.52	4.48	4.49	4.55	4.44	4.07	4.14
3A	3.10	3.11	3.11	3.44	3.39	3.39	3.46	3.54	3.50	3.20
4A	2.34	2.35	2.35	2.67	2.62	2.62	2.68	2.76	3.04	2.54
5A	1.81	1.82	1.82	2.13	2.09	2.08	2.14	2.22	2.50	1.84
α-2T	3.92	3.93	3.93	4.09	4.11	4.10	4.14	4.17	4.26	4.11
α-3T	3.14	3.15	3.15	3.33	3.34	3.34	3.38	3.42	3.57	3.49
α-4T	2.66	2.67	2.67	2.89	2.89	2.89	2.94	3.00	3.18	3.18
α-5T	2.33	2.34	2.34	2.61	2.59	2.59	2.65	2.73	2.95	2.98
α-6T	2.09	2.09	2.09	2.41	2.38	2.39	2.45	2.56	2.83	2.87
Inorganic Semiconductors										
LiF	8.31	8.43	8.53	9.61	9.83	9.71	9.96	10.07	11.41	11.60
LiCl	7.18	7.42	7.54	8.00	8.11	8.27	8.37	8.67	9.35	9.40
NaCl	6.42	6.62	6.78	7.28	7.40	7.59	7.64	8.11	8.81	8.97
LiBr	6.14	6.34	6.52	6.81	6.89	7.12	7.12	7.54	7.70	7.60
NaBr	5.73	5.94	6.12	6.46	6.56	6.79	6.82	7.36	7.54	7.50
MgO	4.21	4.46	4.56	5.25	5.41	5.47	5.67	5.47	6.32	6.21
MgS	1.95	2.07	2.19	2.69	2.83	2.99	3.02	3.14	4.55	4.78
MgSe(ZB)	1.61	1.71	1.75	2.27	2.40	2.50	2.55	2.69	3.75	3.90
MgSe(RS)	2.31	2.51	2.60	2.91	2.99	3.19	3.23	3.22	3.96	3.81
ZnS	2.41	2.50	2.52	3.11	3.26	3.32	3.39	3.44	4.01	3.78
ZnO	1.16	1.19	1.23	1.96	2.14	2.14	2.25	1.86	3.62	3.44
ZnSe	2.09	2.17	2.15	2.78	2.93	2.91	3.04	3.25	2.91	2.82
GeS	1.04	1.09	1.07	1.41	1.49	1.45	1.53	1.13	1.57	1.55
MAE	1.26	1.17	1.12	0.78	0.71	0.65	0.61	0.56	0.11	
MaxAE	3.29	3.17	3.07	2.09	1.95	1.89	1.76	1.64	0.23	

Table S5.

Δ-SCF/DFT and bt-PNO-STEOM-CC/CBS calculated fundamental band gaps ($\Delta E_{F}^{IP \rightarrow EA}$, eV). Statistical evaluation of all quantities is given by means of mean absolute error (MAE) and maximum absolute error (MaxAE).

	BP86	BLYP	PBE	B1LYP	B3LYP	B3PW91	PBE0	B2PLYP	STEOM-CC	Experiment
					Organic Semiconductors					
2A	6.98	8.54	8.32	8.36	8.3	8.33	8.39	8.11	8.19	8.16
3A	6.97	7.5	6.67	6.69	6.65	6.67	6.74	7.78	6.87	6.51
4A	6.97	6.33	5.54	5.55	5.52	5.53	5.58	5.59	5.51	5.39
5A	6.98	5.49	4.72	4.73	4.7	4.71	4.74	5.28	4.8	4.58
α-2T	7.37	7.00	8.52	7.49	7.55	7.50	7.50	7.50	7.60	7.70
α-3T	7.01	7.1	6.19	6.22	6.18	6.22	6.26	6.31	6.44	6.01
α-4T	7.23	6.29	5.42	5.43	5.41	5.45	5.55	5.58	5.4	5.19
α-5T	7.22	5.77	4.92	4.91	4.89	4.95	5.1	5.95	4.8	4.63
α-6T	7.28	5.4	4.56	4.54	4.53	4.59	4.8	4.6	4.31	4.23
					Inorganic Semiconductors					
LiF	9.89	9.61	9.52	11.14	10.94	10.86	11.00	11.99	12.76	13.10
MgO	5.96	5.43	5.9	6.95	6.84	6.85	6.99	7.34	7.18	7.30
MAE	1.75	1.29	0.61	0.38	0.38	0.42	0.45	0.54	0.22	
MaxAE	1.64	1.26	0.60	0.37	0.37	0.40	0.43	0.54	0.22	

IV. Representative Inputs

1) TD-DFT

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 end
%MaxCore 12000

%tddft
  DoSOC true
  Triplets true
  MaxIter 500
  NRoots 100
  PrintLevel 3
end


%pointcharges "file.pc"


*xyz 0 1
Li   28.21236   28.21236   28.21236
Cl   28.21236   28.21236   30.77712
Cl   25.64760   28.21236   28.21236
Cl   28.21236   25.64760   28.21236
Li   28.21236   25.64760   30.77712
Li   25.64760   28.21236   30.77712
Cl   25.64760   25.64760   30.77712
Li   25.64760   25.64760   28.21236
Li> 0.95   25.64760   28.21236   25.64760  NewECP "SDD" end
Li> 0.95   28.21236   25.64760   25.64760  NewECP "SDD" end
Li> 0.95   25.64760   25.64760   33.34188  NewECP "SDD" end
Li> 0.95   28.21236   28.21236   33.34188  NewECP "SDD" end
Li> 0.95   28.21236   23.08284   28.21236  NewECP "SDD" end
Li> 0.95   25.64760   23.08284   30.77712  NewECP "SDD" end
```

```
Li> 0.95   25.64760   30.77712   28.21236  NewECP "SDD" end
Li> 0.95   28.21236   30.77712   30.77712  NewECP "SDD" end
Li> 0.95   23.08284   28.21236   28.21236  NewECP "SDD" end
Li> 0.95   23.08284   25.64760   30.77712  NewECP "SDD" end
Li> 0.95   30.77712   25.64760   28.21236  NewECP "SDD" end
Li> 0.95   30.77712   28.21236   30.77712  NewECP "SDD" end
*
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2) bt-STEOM-CCSD

```
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%maxcore 12000

%mdci
  SteomSOC true
  iroot 1
  MaxIter 500
  nRoots 10
  PrintLevel 3
  DoLeft true
  DoTDM true
  NDav 50
  DTol 1e-4
  DLPNOLINEAR true
  NEWDOMAINS true
  DoEOMMP2 true
  DoRECAN true
end


%pointcharges "file.pc"


*xyz 0 1
Li   28.21236   28.21236   28.21236
Cl   28.21236   28.21236   30.77712
Cl   25.64760   28.21236   28.21236
Cl   28.21236   25.64760   28.21236
Li   28.21236   25.64760   30.77712
Li   25.64760   28.21236   30.77712
Cl   25.64760   25.64760   30.77712
Li   25.64760   25.64760   28.21236
Li> 0.95   25.64760   28.21236   25.64760  NewECP "SDD" end
Li> 0.95   28.21236   25.64760   25.64760  NewECP "SDD" end
Li> 0.95   25.64760   25.64760   33.34188  NewECP "SDD" end
Li> 0.95   28.21236   28.21236   33.34188  NewECP "SDD" end
Li> 0.95   28.21236   23.08284   28.21236  NewECP "SDD" end
Li> 0.95   25.64760   23.08284   30.77712  NewECP "SDD" end
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Li> 0.95   25.64760   30.77712   28.21236  NewECP "SDD" end
Li> 0.95   28.21236   30.77712   30.77712  NewECP "SDD" end
Li> 0.95   23.08284   28.21236   28.21236  NewECP "SDD" end
Li> 0.95   23.08284   25.64760   30.77712  NewECP "SDD" end
Li> 0.95   30.77712   25.64760   28.21236  NewECP "SDD" end
Li> 0.95   30.77712   28.21236   30.77712  NewECP "SDD" end
*
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3) Pointcharges file (file.pc)

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-0.95  51.29520    0.00000    0.00000
-0.95  51.29520    0.00000   51.29520
-0.95  51.29520   51.29520    0.00000
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V. References

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