NSCI SI2-SSE: Multiscale Software for Quantum Simulations of Nanostructured Materials and Devices

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- **"Real" materials structures are often complex and cannot be reduced to a few hundreds of atoms**
  - **Process simulation requires large systems**
- **Materials Genome – White House initiative to "deploy advanced materials twice as fast, at a fraction of the cost"**
- **National Strategic Computing Initiative (NSCI)**
- **National Quantum Initiative - multi-agency program in QIS: NSF, DOE**
- **Real-space multigrid (RMG) open-source software www.rmgdft.org**
  - **Can simulate quantum materials and devices on the latest pre-exascale and exascale multi-core/multi-GPU supercomputers, e.g., the IBM-NVIDIA Summit. Scales from desktops to supercomputers.**

Reproducibility of DFT calculations for solids

RMG vs Win2K
Accurate and reliable

H 1.852																	He ---
Li ---	Be 0.831											B ---	C 0.047	N 4.558	O ---	F ---	Ne ---
Na ---	Mg 0.492											Al ---	Si 0.407	P 0.502	S ---	Cl 0.259	Ar ---
K 0.010	Ca 0.105	Sc 0.260	Ti 0.107	V 0.582	Cr 1.749	Mn 2.146	Fe 2.203	Co 0.173	Ni 0.378	Cu 0.927	Zn 0.031	Ga 0.214	Ge 0.577	As 1.656	Se 0.055	Br 0.886	Kr ---
Rb 0.111	Sr 0.184	Y 0.177	Zr 0.081	Nb 1.108	Mo 1.025	Tc 0.731	Ru 1.417	Rh 1.689	Pd 1.638	Ag 0.675	Cd 0.818	In 0.290	Sn 0.417	Sb ---	Te 0.406	I 0.096	Xe ---
Cs 0.031	Ba 0.353	Lu ---	Hf 1.408	Ta 0.735	W 0.489	Re 0.618	Os 1.439	Ir 0.713	Pt 0.905	Au 1.559	Hg 0.056	Tl 0.037	Pb 1.010	Bi ---	Po ---	At ---	Rn ---

- **New features:**
  - **Hybrid functionals**
  - **Non-collinear spin**
  - **Spin-orbit coupling**

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