

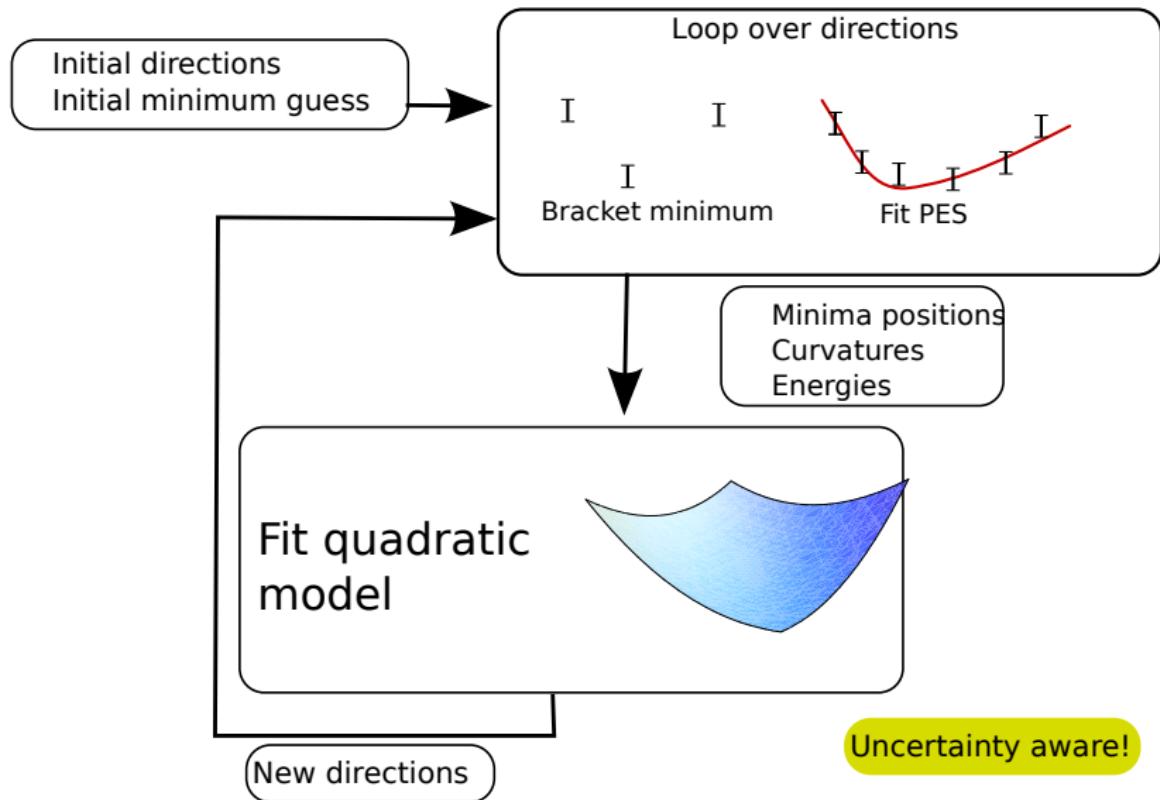
Open source quantum Monte Carlo and an application to metal hydride clusters

Lucas K. Wagner

Materials Science & Engineering
Massachusetts Institute of Technology

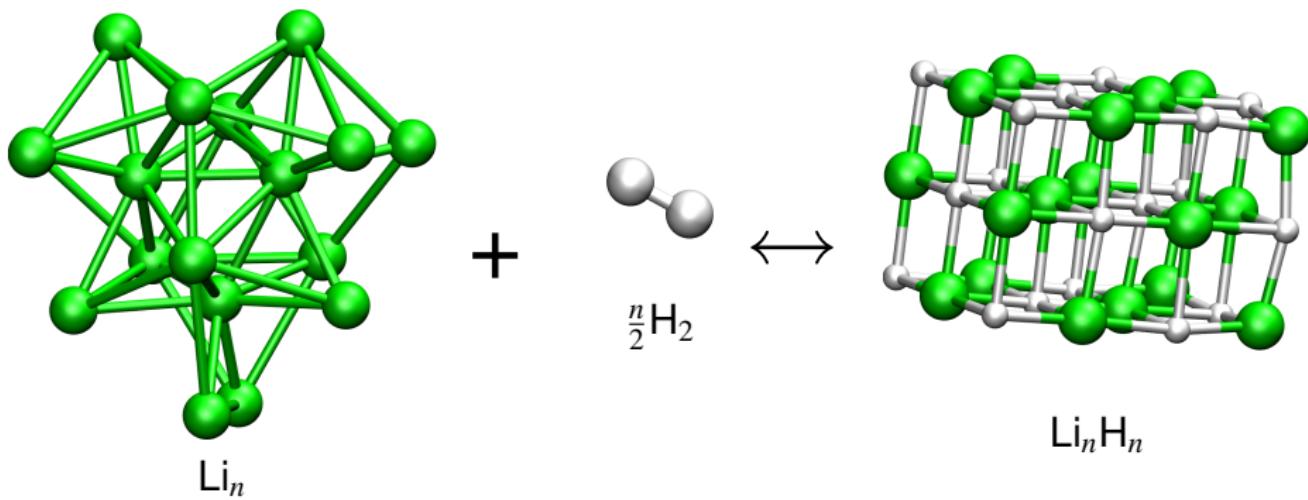
In collaboration with Jeffrey Grossman (MIT), Eric Mazjoub (UC-Davis), and Mark Allendorf (Sandia Livermore)

Phys. Rev. Lett. **104** 210201 (2010)
September Psi-K meeting



QWalk

(15 minutes)



QWalk

<http://www.qwalk.org>

J. Comp. Phys. **228** 3390

Hamiltonian

Molecules
1-D rings

Solids

Electron gas
All-electron

Pseudopotentials

Wave function

Multiple determinants
Pfaffians

Flexible Jastrow

Twisted BC's
Pfaffians+Backflow

Backflow
Method

DMC
Energy minimization

RMC

VMC
T-moves

Self-healing

GAMESS
SIESTA

Interfaces

ABINIT
CRYSTAL

GAUSSIAN

QWalk

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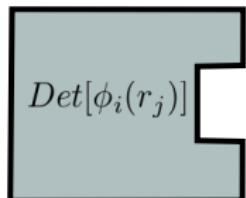
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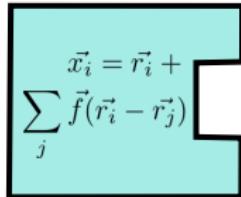
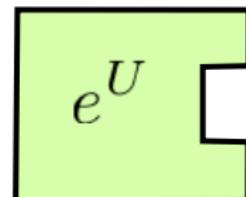
GAUSSIAN



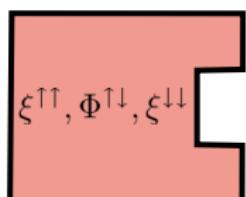
Wave function calculator



Slater Determinant **Jastrow factor**



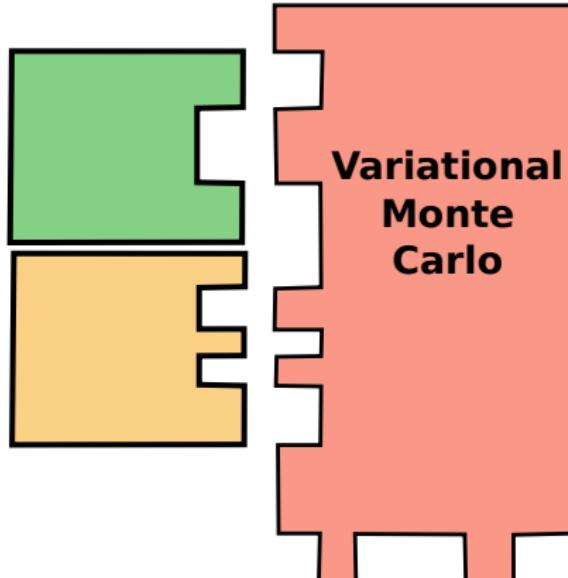
Backflow



Pfaffian

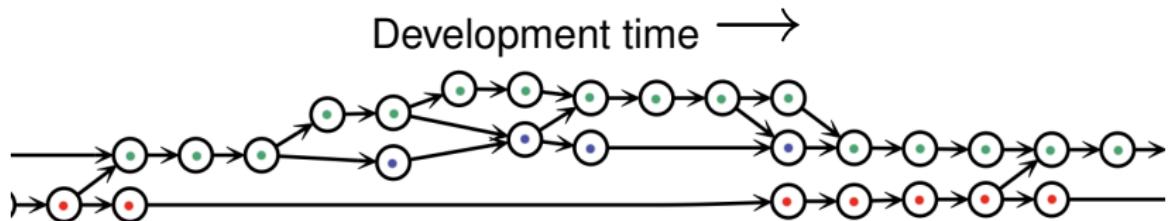
**Wave
function
calculator**

**Potential
energy
calculator**



**Variational
Monte
Carlo**

**Method
interface**



Using Mercurial (<http://mercurial.selenic.com/>)

Code contributed by

Michal Bajdich

Shuming Hu

Jindrich Kolorenc

Kevin Rasch

Pavel Vagner

Rene Derian

Paul Kent

Jarrod McClean

Fernando Reboreda

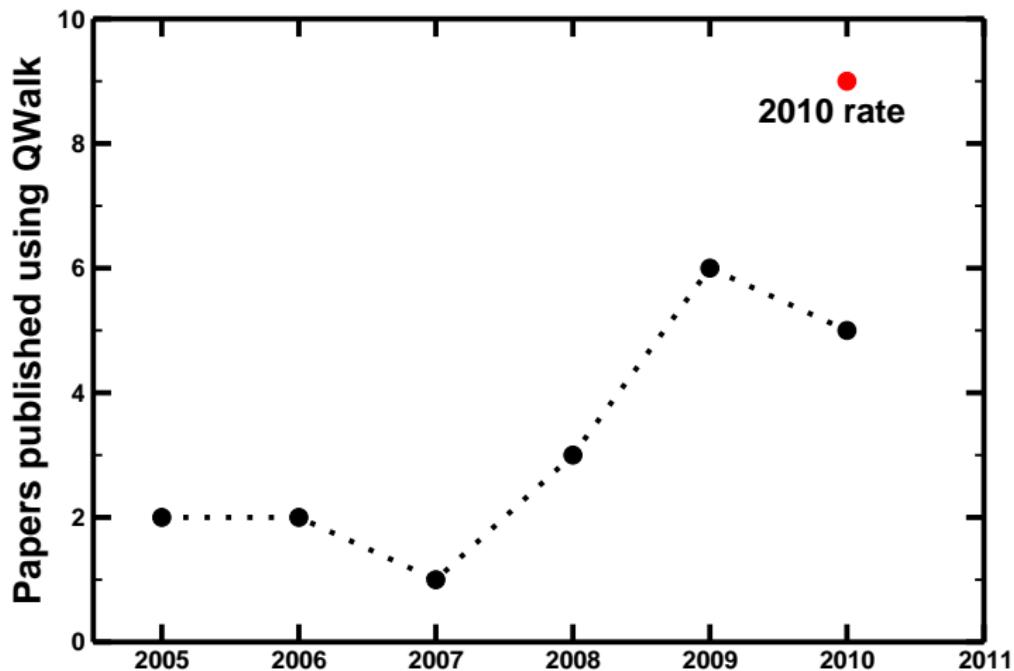
Lucas Wagner

Zachary Helms

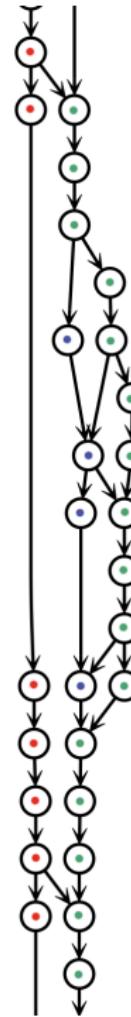
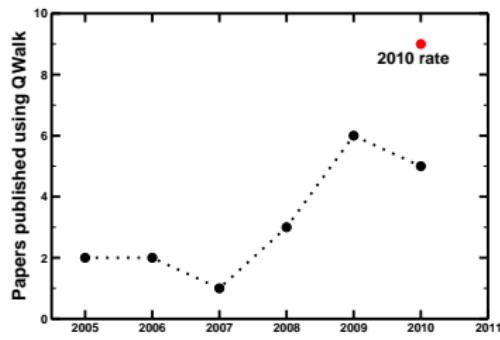
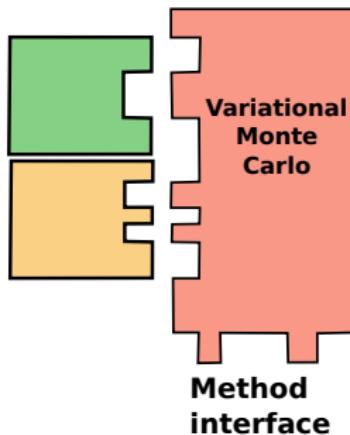
Hiori Kino

Lubos Mitas

David Sulock



Wave
function
calculator
Potential
energy
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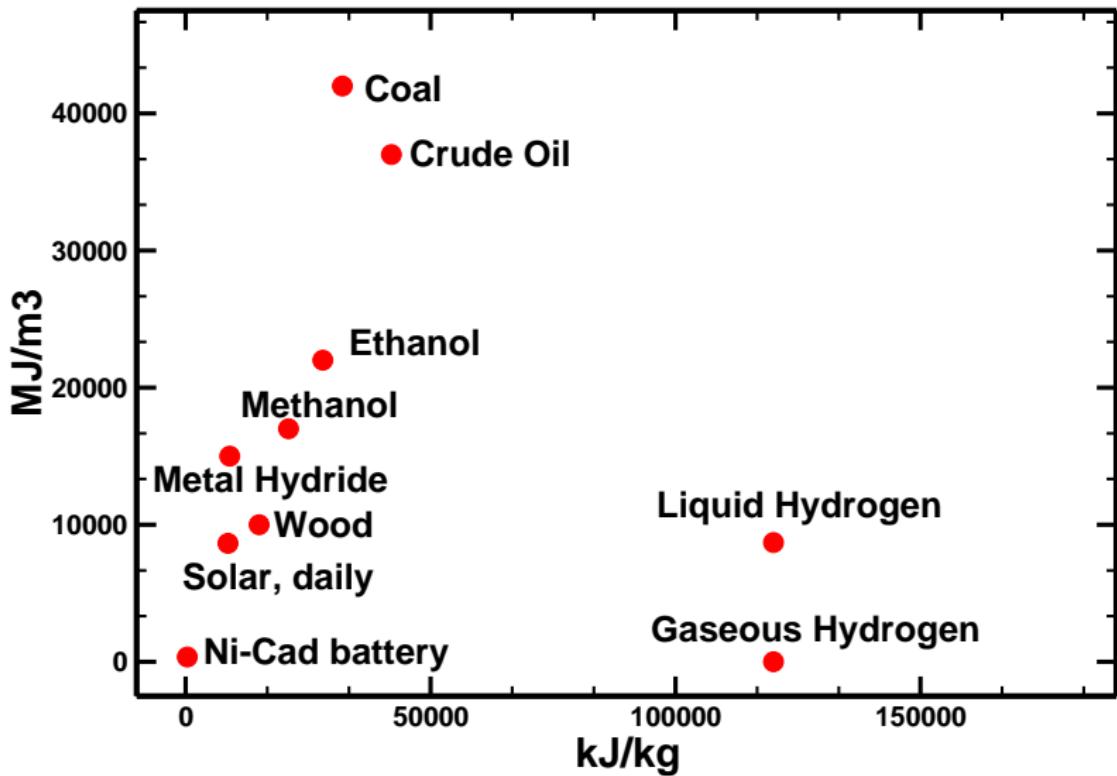
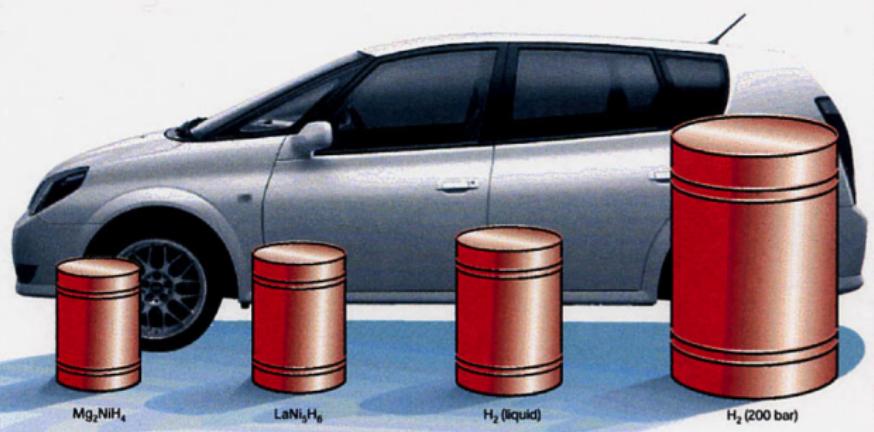
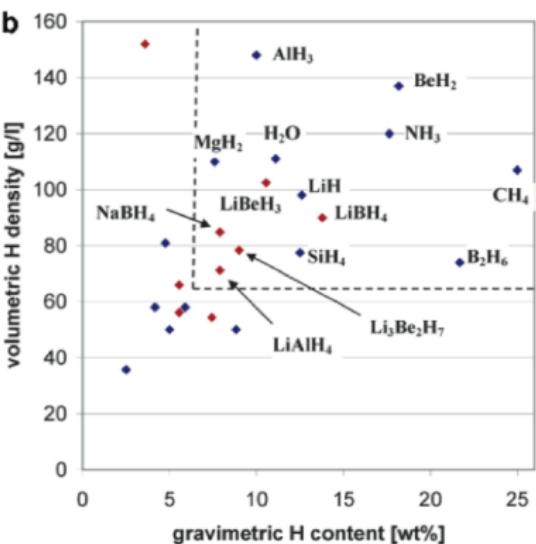


Figure 1 Volume of 4 kg of hydrogen compacted in different ways, with size relative to the size of a car. (Image of car courtesy of Toyota press information, 33rd Tokyo Motor Show, 1999.)

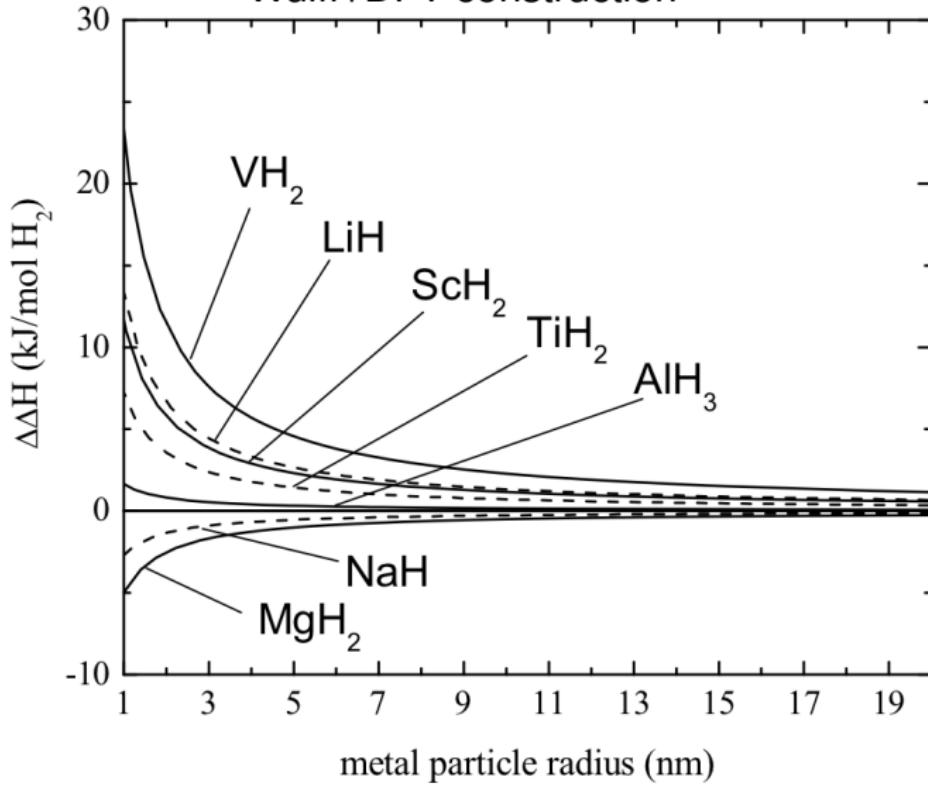


a

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18			
I	H																He			
Li	Be																Ne			
Na	Mg																Ar			
K	Ca	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36			
Rb	Sr	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr			
Cs	Ba	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	54		
Fr	Ra	55	56	*	71	72	73	74	75	76	77	78	79	80	81	82	83	86		
		87	88	**	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
				*	Lr	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo
				**	57	58	59	60	61	62	63	64	65	66	67	68	69	70		
					La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb		
					89	90	91	92	93	94	95	96	97	98	99	100	101	102		
					Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	Nb		

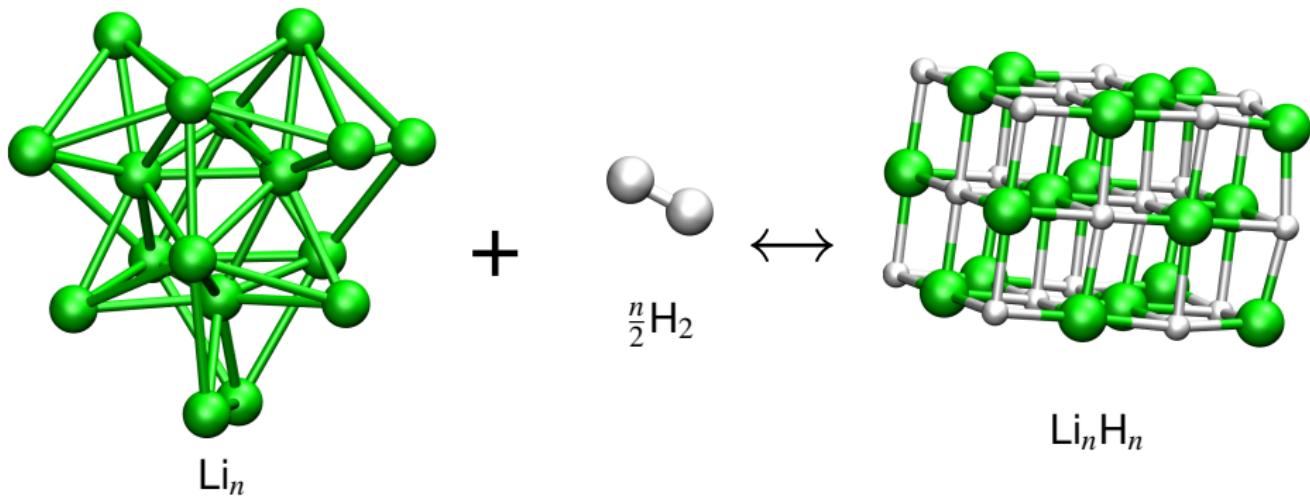


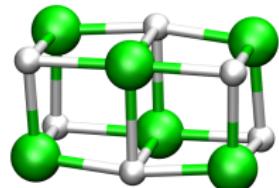
Wulff+DFT construction¹



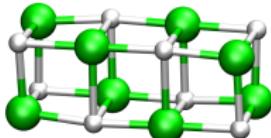
¹Kim, Dai, Johnson and Sholl, Nanotechnology, 20, 204001

- ▶ Codes: NWChem, GAMESS, CRYSTAL, QWalk.
- ▶ cc-TZP basis
- ▶ cusp corrections, angular Green's function (UNR), timestep $0.01 \text{ Hartrees}^{-1}$.
- ▶ QMC: Slater-Jastrow w/ B3LYP geometries & orbitals

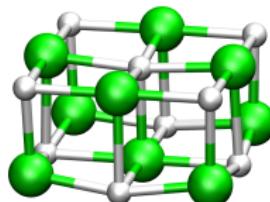




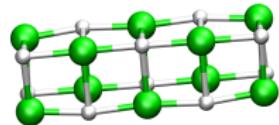
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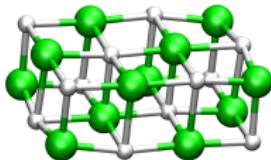
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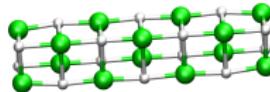
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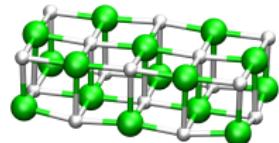
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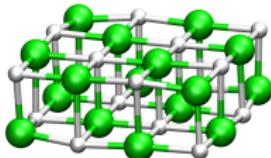
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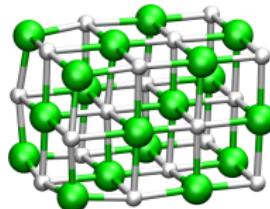
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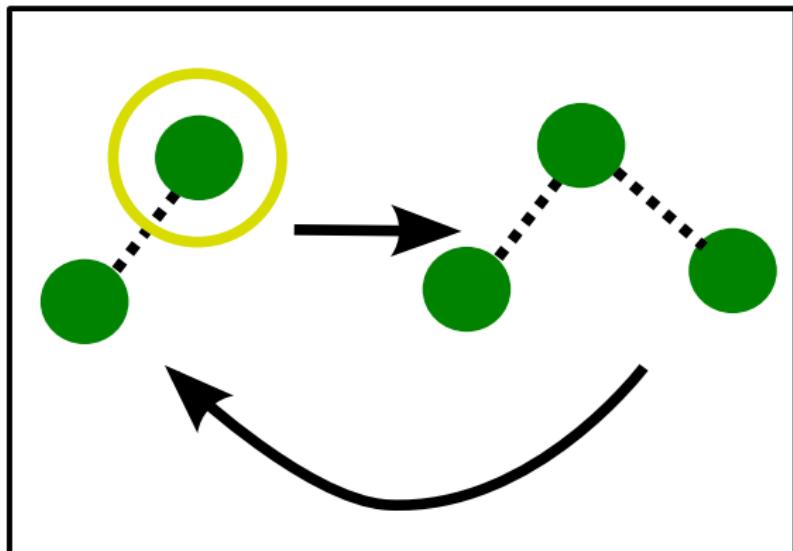
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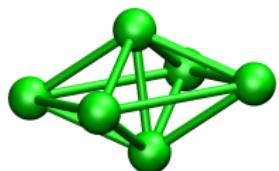


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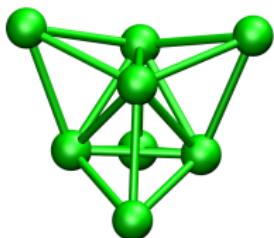


Candidate structure

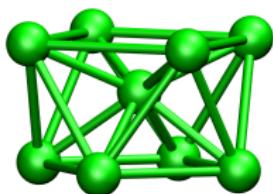
DFT-B3LYP optimization



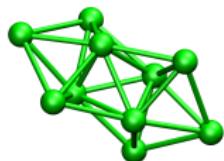
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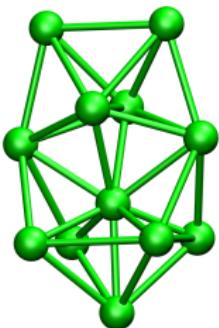
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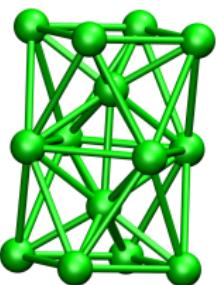
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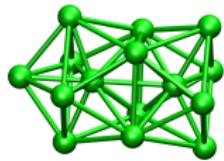
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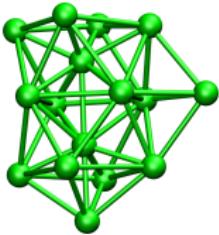
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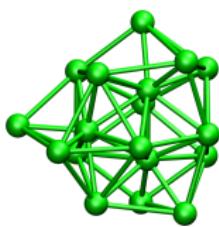
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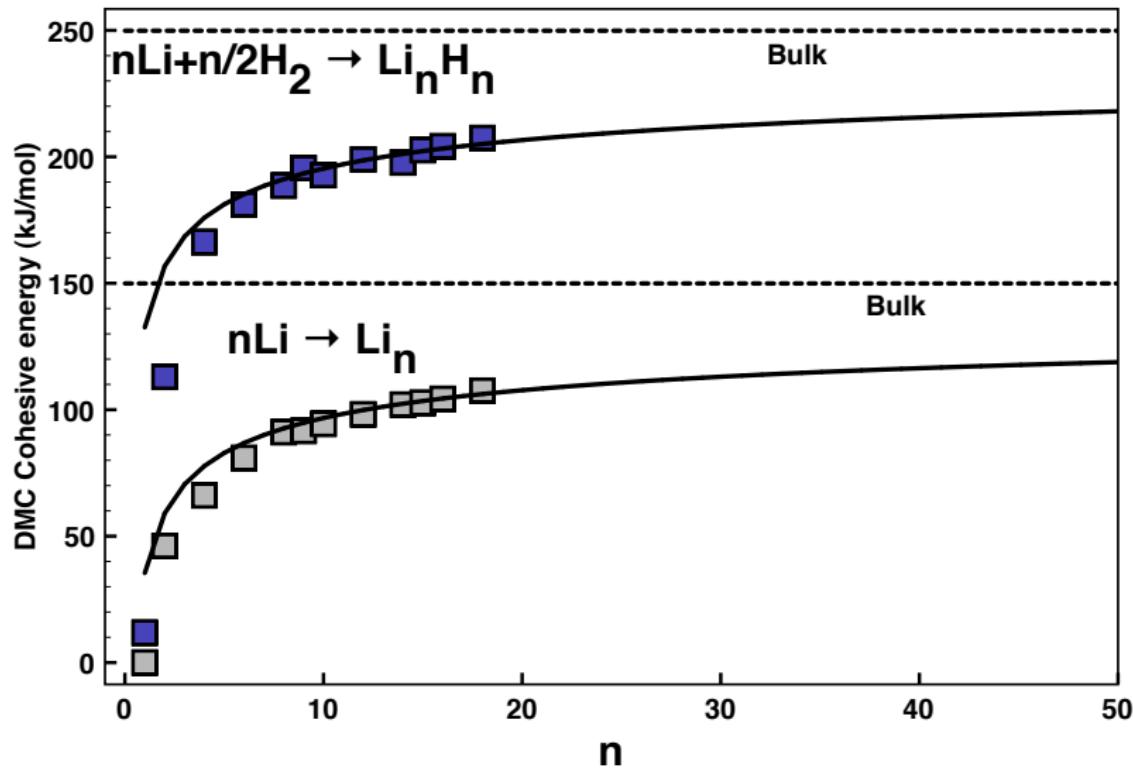
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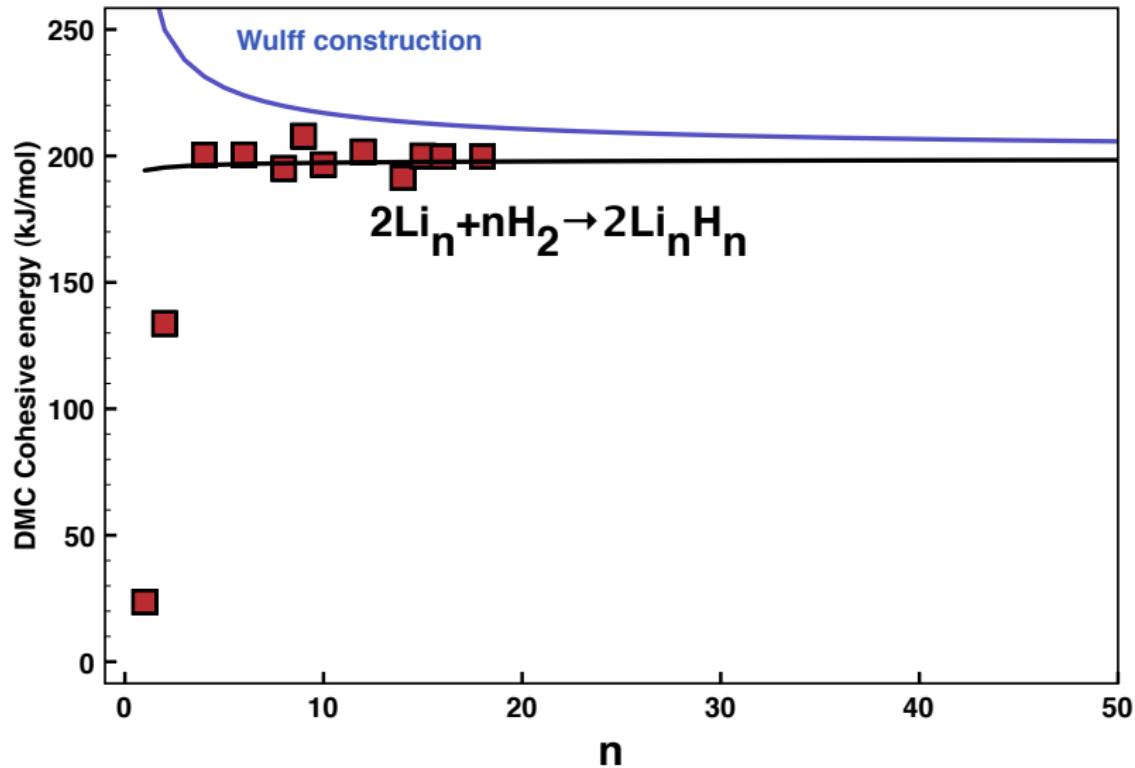
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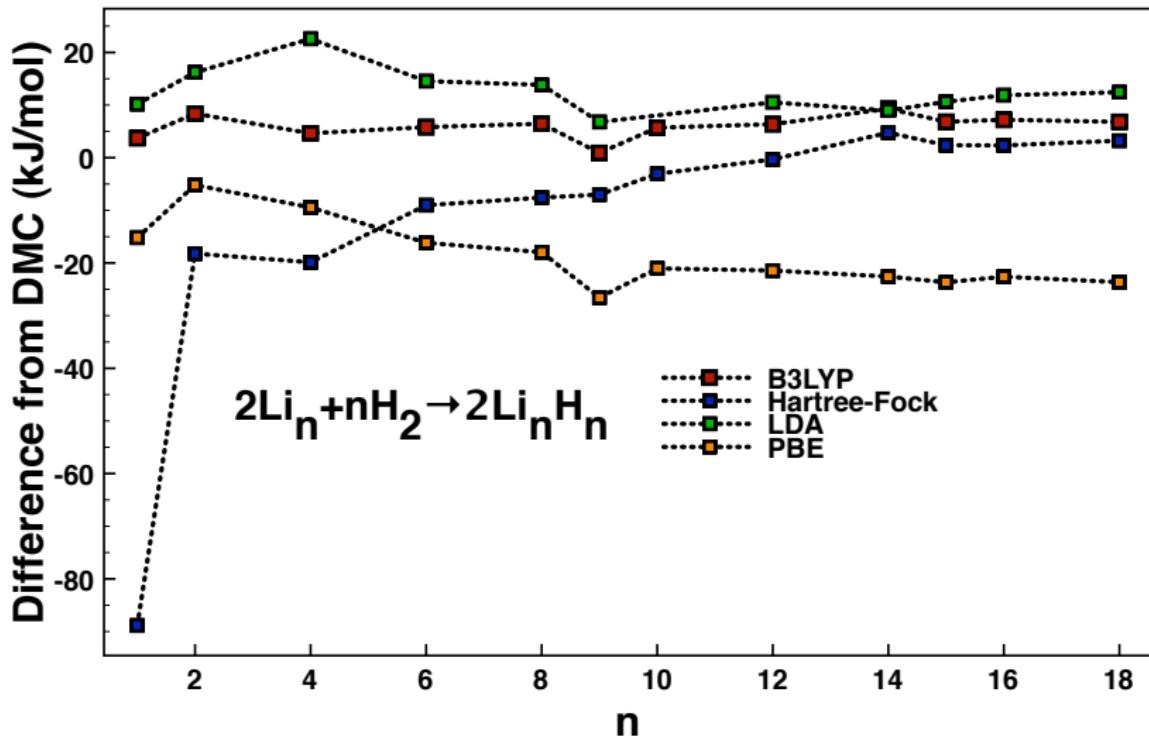


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$$\text{Fit: } E_{coh}(n) = E_{coh}(\text{bulk}) + \alpha/n^{1/3}$$





PBE differences

