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Implementation of the LDA-1/2 method in ABINIT

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ABINIT Developper Workshop, Louvain-La Neuve - May 20th, 2019

The LDA-1/2 method

Objective: improve the description of band gaps

Method: LDA-1/2 , derived from the Slater-Janack transition state theory

Theorem of Janack: $\frac{\partial E}{\partial f_\alpha} = e_\alpha(f_\alpha)$

e_α: eigen value of the Kohn-Sham state α

f_α: occupation of the Kohn-Sham state α

It can be shown that: $e_\alpha(0) - e_\alpha\left(-\frac{1}{2}\right) = S_\alpha$

with $S_\alpha = \int n_\alpha(\vec{r}) V_S(\vec{r}) d^3r$, the hole self-energy

and

$$E(0) - E(-1) = e_\alpha(0) - S_\alpha$$

band gap

L. G. Ferreira et al., Phys. Rev. B, 78, 125116 (2008)

The LDA-1/2 method

It can then be shown that:

$$V_S = V(0,r) - V(-\frac{1}{2},r)$$

This is an atomic formulation. In a cristal, the self-energy potential is cut with:

$$\Theta(r) = \left[1 - \left(\frac{r}{CUT}\right)^8\right]^3$$

If r< CUT, 0 otherwise.

In ATOMPAW:

- first calculation with the neutral atom configuration → V(0,r)
- Second calculation on ion without ½ electron → V(-1/2, r)
- Calculation of V_S.
- a new tag « LDA_minus_half_potential » is inserted in the JTH XML PAW data files for 10 elements

TABLE III. Values of *CUT* that make the band gaps extreme, that is, when the self-energy potential is defined by Eq. (18) and trimmed by Eq. (22). The optimal value of *CUT*, as is the case of an ionic or covalent radius, is typical of each atom and the orbital that was half ionized. In most cases only the anion matters.

Atom	Half ionized Orbital	*CUT* (a.u.)
Si	*p*	3.67
N	*p*	2.90
As	*p*	3.81
O	*p*	2.67
Ga	*d*	1.23
Ge	*p*	3.46
P	*p*	3.86
Zn	*d*	1.665
S	*p*	3.39
In	*d*	2.126

TABLE IV. Band energy gaps (eV) for several semiconductors obtained with the LDA-1/2 at experimental lattice constant, by using the VASP code and SIESTA (S), compared with pure LDA, GW, and experimental results in Ref. 32 except where noted. Direct energy gaps are denoted as (d) and the indirect ones as (i). The majority of the LDA-1/2 calculations were obtained using only the trimmed self-energy potential of *p* anion; exceptions are noted.

	LDA-1/2	LDA	Expt.	GW
C (i)	5.25 (S)[a]	4.13	5.47[b]	5.48–5.77[c]
C (d)	6.75 (S)[a]	5.54	7.3[b]	
Si (i)	1.137, 1.21 (S)	0.51	1.17[b]	1.32,[d] 0.95–1.10[c]
Si (d)	2.9, 2.94 (S)	2.54	3.05, 3.40[b]	
Ge (i)	0.70	0.08	0.66–0.74[b]	0.66–0.83[c]
AlN (d)	6.06	4.27	6.23	5.83–6.24[c]
GaN (d)	3.52[e]	1.95	3.507	3.15–3.47[c]
InN (d)	0.95[e]	–0.29	0.7–1.9	0.20–0.33[c]
AlP (i)	2.79	1.47	2.52	2.59[d]
GaP (i)	2.36($\Gamma-L$) [e]	1.49($\Gamma-X$)	2.35	2.55[d]
InP (d)	1.12[e]	0.50	1.42	1.44[d]
AlAs (i)	2.73	1.34	2.24	2.15[d]
GaAs (d)	1.41	0.41	1.519	1.22,[d] 1.40–1.70[c]
InAs (d)	0.75	–0.34	0.417	0.31[d]
ZnO (d)	3.29[e]	0.83	3.4[b]	2.51–3.07[c]
ZnS (d)	3.68[e]	2.02	3.91[b]	3.21–3.57[c]

IMPLEMENTATION

In ABINIT:

- V_S is treated as an external potential.

- $E_{ext} = \int d\boldsymbol{r}\tilde{n}(\boldsymbol{r})v_{ext}(\boldsymbol{r}) + \sum_a \int d\boldsymbol{r}[n^a(\boldsymbol{r}) - \tilde{n}^a(\boldsymbol{r})]v_{ext}(\boldsymbol{r})$

- $H = v_{ext} + \sum_{i,j} |\tilde{p}_j > D_{i,j} < \tilde{p}_i|$ with $D_{i,j} = \int d\boldsymbol{r} v_{ext}(\boldsymbol{r})\left[\phi_i(\boldsymbol{r})\phi_j(\boldsymbol{r}) - \tilde{\phi}_i(\boldsymbol{r})\tilde{\phi}_j(\boldsymbol{r})\right]$

- The **ldaminushalf** input variable must be set to 1

Example: indirect gap of silicon: LDA → 0.55 eV
LDA-1/2 → 1.25 eV