ON-SITE APPROXIMATION FOR SPIN-ORBIT COUPLING IN LCAO DENSITY FUNCTIONAL METHODS: APPLICATION TO CLUSTERS AND CHAINS

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We propose a computational method that simplifies drastically the inclusion of spin-orbit interaction in density functional theory implemented on localised atomic orbital basis sets. Our method is based on a well-known procedure for obtaining pseudopotentials from atomic relativistic ab initio calculations and on an on-site approximation for the spin-orbit matrix elements. We have implemented the technique in the SIESTA code[1], and we show that it provides accurate results for the overall band structure and splittings of group IV and III-IV semiconductors as well as for 5d metals[2]. We also analyze the impact of the magnetic anisotropy on the geometric structure and magnetic ordering of small atomic clusters of palladium, iridium, platinum and gold[3]. Our results highlight the absolute need to include self-consistently the spin orbit interaction in any simulation of the magnetic properties of small atomic clusters, and a complete lack of universality in the magnetic anisotropy of small-sized atomic clusters.

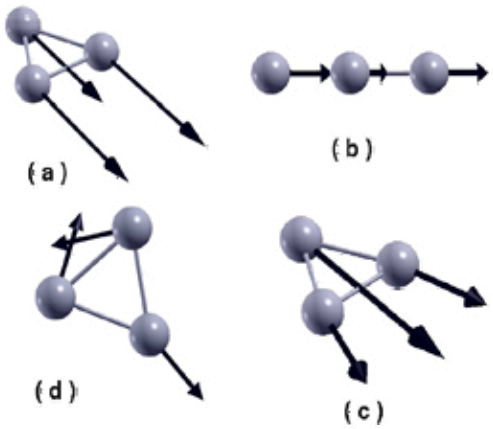
References:

[1] cond-mat/0611624 Predictions for the formation of new atomic chains in Mechanically Controllable Break Junction experiments. Lucas Fernandez Seivane, Victor M. Garcia-Suarez, Jaime Ferrer. *Phys. Rev. B* **75**, 075415 (2007).
[2] cond-mat/0610879 Magnetic anisotropies of late transition metal atomic clusters. Lucas Fernandez Seivane, Jaime Ferrer. Physical Review Letters **99**, 183401 (2007)
[3] cond-mat/0601093 On-site approximation for spin-orbit coupling in LCAO density functional methods. Lucas Fernandez Seivane, Miguel A. Oliveira, Stefano Sanvito, Jaime Ferrer. *J. Phys.: Condens. Matter* 18 7999-8013, 2006.
[4] M. N. Huda, M. K. Niranjan, B. R. Sahu and L. Kleinman, *Phys. Rev. A* 73, 053201 (2006).
[5] F. Aguilera-Granja, J. Ferrer and A. Vega, *Phys. Rev. B*, 74 174416 (2006).

Figures:

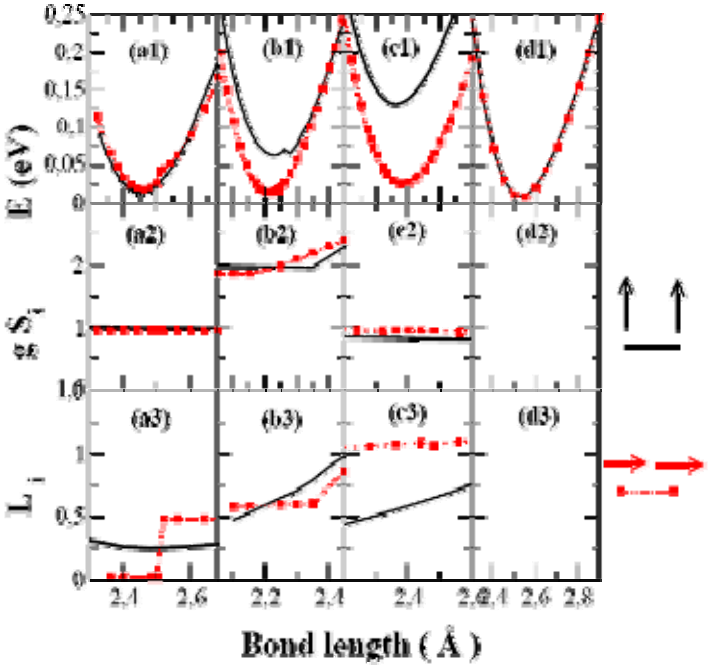
Results for Trimers

Equilibrium geometries and spin moments $g \cdot S_i$ of (a) Pd_3, (b) Ir_3, (c) Pt_3 and (d) Au_3.



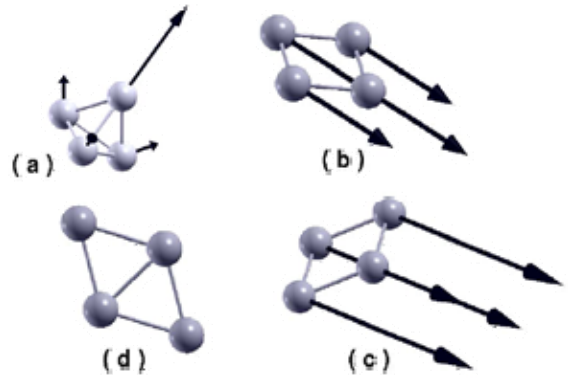
Left to right: (a) Pd2, (b) Ir2, (c) Pt2 and (d) Au2.

Up downwards: (1) Energy, (2) Spin moment per atom times gyromacnetic ratio and (3) Orbital angular moment per atom



Results for Tetramers

Equilibrium geometries and spin moments $g \cdot S_i$ of (a) Pd_4, (b) Ir_4, (c) Pt_4 and (d) Au_4.



Results for Pentamers

Equilibrium geometries and spin moments $g \cdot S_i$ of (a) Pd_5, (b) Ir_5, (c) Pt_5 and (d) Au_5.