# SPIN-ORBIT COUPLING IN SOLIDS, MOLECULES AND CLUSTERS WITH LCAO METHODS

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Relativistic corrections in *ab initio* calculations are usually included using the scalar relativistic approximation[1, 2] which contains the effect of the mass shift and the Darwin term. The remaining term, the spin-orbit coupling, is a short-range non-local interaction expressed as:

$$\hat{V}^{SO} = \sum_{l,m} |l,m\rangle V_l^{SO}(\vec{r})\vec{L}\cdot\vec{S}\langle l,m|,$$

where $V_l^{SO}$ is an average difference of the relativistic calculated pseudopotentials $V_{l\pm1/2}$.

Possible approaches to deal with this spin-orbit interaction in *ab initio* calculations are:

1) to completely neglect it
2) to treat it as a perturbation,[3] or
3) to use alternative Kleynman-Bylander decompositions.[3]

In *ab initio* LCAO calculations the spin-orbit term is usually neglected as it generates three center integrals which are prohibitively expensive to compute. However this term originates deep in the core region and for this reason overlaps should only be appreciable if calculated "on-site".

We have thus considered an "on-site" approximation to the spin-orbit coupling term that we have implemented in the code SIESTA.[4] The matrix elements are now only one center integrals which require very little computational overhead.

Results for III-V semiconductors, bulk metals, atomic clusters (5d) and selected molecules are computed and compared with experimental values. These show good agreement demonstrating the possibility of performing accurate *ab initio* spin-orbit calculations without heavy computational costs.

**References:**

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[2] G. B. Bachelet and M. Schlüter, Physical Review B 25, 2103 (1982).
[3] L. A. Hemstreet, C. Y. Fong, and J. S. Nelson, Physical Review B 47, 4238 (1993).
[4] J. M. Soler et al., Journal of Physics: Condensed Matter 14, 2745 (2002).