

### Inclusion of spin-orbit coupling in recursion method

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**Abstract:** The discussion of stability properties of alloys of heavier elements requires the inclusion of relativistic corrections to standard electronic structure calculation. It was argued by Singh [1] and Paudyalet. al [2] that unless one include at least the scalar relativistic corrections for NiPt, one cannot predict the observed low temperature ordering in the 25 %, 50 % and 75 % composition alloys. Scalar relativistic corrections e.g. Mass-velocity corrections and Darwin corrections are now routinely incorporated in most electronic structure calculations for both ordered compounds as well as disordered alloys. The inclusion of Spin-orbit coupling has been less common. We presented the methodology for including spin-orbit coupling in ordered system.

In many-electron systems the spin-orbit Hamiltonian can be written as,

$$H_{SO} = \frac{1}{c^2} \frac{1}{r} \frac{dV(r)}{dr} \vec{L} \cdot \vec{S} = v(r) \vec{L} \cdot \vec{S} \quad (1)$$

As in earlier communication [3], we shall use the self-consistently compound LSDA potential in an atomic sphere for the potential V(r). We shall use the spherically averaged form as in standard LMTO approaches, although this restriction may be relaxed. We shall use the spherically averaged form, as in standard LMTO approaches, although this restriction may be relaxed. We shall also use inflated atomic spheres and neglect contributions from the interstitial regions. The use of the LSDA potential in H<sub>SO</sub> has really no formal justification. Stiles et. al. [4] have argued that a more systematic approach should be incorporate, within the Hamiltonian, two-body terms of the kind introduced by Breit [5]. This would require corrections to the Hartree energy of the form;

$$E_{SO} = \frac{\alpha^2 E_h a_0^3}{4} \int d^3\vec{r} \int d^3\vec{r}' \left\{ n(\vec{r}) \vec{d}(\vec{r}) \cdot \frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|^3} - 2\vec{j}(\vec{r}) \cdot \vec{m}(\vec{r}') \times \frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|^3} \right\} \quad (2)$$

Where  $\alpha \cong 1/137$ ,  $E_h = 27.21$  eV and  $a_0 = 0.529$  nm and,

$$n(\vec{r}) = \sum_{i \in OCC, \sigma} \psi_{i\sigma}^*(\vec{r}) \psi_{i\sigma}(\vec{r})$$

$$\vec{j}(\vec{r}) = i \sum_{i \in OCC, \sigma} \psi_{i\sigma}^*(\vec{r}) \vec{\nabla} \psi_{i\sigma}(\vec{r})$$

$$\vec{m}(\vec{r}) = \sum_{i \in \text{occ}, \sigma} \psi_{i\sigma}^*(\vec{r}) \vec{\sigma} \psi_{i\sigma}(\vec{r})$$

$$\vec{d}(\vec{r}) = \psi_{i\sigma}^*(\vec{r}) \vec{\sigma} \times \vec{\nabla} \psi_{i\sigma}(\vec{r})$$

The variational derivative of the above equation (2) with respect to the wave function would yield the effective spin-orbit term that enters the Kohn-Sham equation as  $H_{\text{SO}}$ . The first term yields the standard spin-orbit term shown by us earlier.

In an earlier communication [3], we observed that spin-orbit coupling play significant role in alloys of the heavier elements. In the same communication, we proposed a methodology for taking into account the spin-orbit coupling in the recursion method for ordered system. The basis used for the representation of the Hamiltonian is the TB-LMTO [6]. Since its sparseness is an essential requirement for recursion. We also extend the model for the rough surfaces. We presented some numerical examples to validate our assumption. The recursion technique [7] can then be extended to augmented space to deal with disordered alloys.

## References

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