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Evidencing the relationship between isomer spectra and melting : the 20- and 55-atom silver and gold clusters cases

Mathias Rapacioli,*[a] Fernand Spiegelman,[a] and Nathalie Tarrat*[b]

[a] Laboratoire de Chimie et Physique Quantiques LCPQ/IRSAMC, UMR5626, Université de Toulouse (UPS) and CNRS, 118 Route de Narbonne, F-31062 Toulouse, France. Tel: 33 5 6155 8318
[b] CEMES, Université de Toulouse, CNRS, 29, rue Jeanne Marvig, 31055 Toulouse, France. Tel: 33 5 6752 4347

Corresponding Authors : mathias.rapacioli@irsamc.ups-tlse.fr ; nathalie.tarrat@cemes.fr

Details about the DFTB parameters used in this work and in the previous ones (1; 2; 3; 4; 5) are given below.

1 Gold parameters

The gold parameters consist in a very slight modification of the parameters published by Fihey *et al.* (auorg set from www.dftb.org website) (6), namely a shift of the p orbital energy from -0.02786 to -0.00001 Ha.

2 Silver parameters

The silver parameters is a modification of the hyb-0-1 set parameter from www.dftb.org website) (7). The modifications consist in :

- a shift of the p orbital energy from -0.02814 to -0.00800 Ha.
- a shift of Hamiltonian and overlap matrices by 0.38 Bohr toward shorter distances and a multiplication of the Hamiltonian matrix elements by 0.9.
- the use of a polynomial repulsive potential following the classical expression

$$\sum_{i=2}^{6} c_i (r_{cut} - r)^i$$

with the polynomial coefficients equal in atomic units to 0.00473661, 1.62067e-05, 0.0121596, -0.0352701, 0.0233099 and r_{cut} to 5.48.

References

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