

## Study of Jahn-Teller effect in solid state impurities through Cluster Model Calculations

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### ABSTRACT

The  $E_g \otimes e_g$  Jahn-Teller effect in impurities in cubic lattices has been studied by means of DFT calculations. This approach has many advantages when compared to previous methods. In particular it allows to calculate parameters of model Hamiltonians *individually* providing a tool for understanding their physical origin and to study which terms in the Hamiltonian have greater importance. This is specially true in order to decide to include second order vibronic coupling or anharmonicity terms.

Three systems have been studied, obtaining very good agreement with experimental data in all of them.  $\text{NaCl}:\text{Rh}^{2+}$  which presents strong Jahn-Teller effect,  $\text{KCl}:\text{Cu}^{2+}$  which presents a large deformation and the series  $\text{MO}:\text{Cu}^{2+}$  (M=Mg, Ca, Sr) which presents the transition from weak (Mg) to strong (Sr) Jahn-Teller effect.

Our results are all coherent with the supposition that the anharmonicity term in the Hamiltonian is more important than the second order vibronic coupling. Also discussion is carried out in order to establish the importance of the coupling of centre to the rest of the lattice.