Development of a wavefunction-based ab initio method for metals applying the method of increments

Beate Paulus, Elena Voloshina, Dirk Andrae

Freie Universität Berlin, Institut für Chemie und Biochemie

Takustr. 3, 14195 Berlin, Germany

Ab initio electron correlation calculations based on quantum-chemical methods are successfully applied to metallic systems via the method of increments. To deal with the two distinct problems that occur in metals, the difficulty of localization of the orbitals and the generation of clusters with neutral atoms in the center, we proposed an embedding scheme which has itself no metallic character but can mimic the metal in the internal region, where the atoms are correlated. The first application was made for solid mercury, where a very good agreement with experimental ground-state properties was achieved. Further the approach has been extended to other group 2 and 12 metals (Be, Mg, Zn, and Cd) where the metallic character is more pronounced than in mercury. Application of the method of increments to the investigated metallic systems allows us not only to obtain values close to experimental data but also to understand the influence of individual correlation-energy increments on cohesive properties and to clarify thereby some aspects of the structural features of the group 12 metals. Ongoing work on the group 2 metals Ca, Sr and Ba as well as on metallic ytterbium is presented.

Literature:

E. Voloshina and B. Paulus, *Wavefunction-based ab initio correlation method for metals: Application of the incremental scheme to* Be, Mg, Zn, Cd, and Hg, in Book Series: Chemical Modelling: Applications and Theory (Specialist Periodical Reports), Vol. 6, M. Springborg (ed.), R.S.C., Cambridge, 2009. (further references therein)