

Recent developments on ES2MS package

Keisuke Hatada¹*, Naoki Komiya², Fukiko Ota², Kaori Niki², Ján Minár³,
Hubert Ebert⁴, Calogero R. Natoli⁵, and Didier Sébilleau⁶

¹*Faculty of Science, University of Toyama, Gofuku 3190, Toyama 930-8555, Japan*

²*Graduate school of Advanced Integration science, Chiba University, Chiba 263-8522, Japan*

³*New Technologies-Research Center, University of West Bohemia, Univerzitní 8, 306 14 Plzeň, Czech Republic*

⁴*Ludwig-Maximilians-Universität München, Department Chemie, Butenandt- str. 5-13, D-81377 München, Germany*

⁵*LNF-INFN, Via E. Fermi 40, 00044, Frascati, Italy*

⁶*Département Matériaux-Nanosciences, Institut de Physique de Rennes, UMR URI-CNRS 6251, Université de Rennes1, 35042 Rennes cedex – France*

Email: * hatada@sci.u-toyama.ac.jp

We present an interface package, called ES2MS[1], for passing self-consistent charge density and potential from Electronic Structure (ES) codes To Multiple Scattering (MS) codes. MS theory is based on the partitioning of the space by atomic-size scattering sites, so that the code provides the charge densities and potentials for each scattering site. For pseudo potential codes, such as VASP[2], the interface solves Poisson equation to construct the all-electron potential on the radial mesh which is used to solve the transition operators (T-matrix) and Green's functions in MS codes. Recently we have further developed the interface for Gaussian09 [3] and SPR-KKR [4]. In the case of Gaussian 09, the Poisson equation is solved by a recurrence relation based on the set of Gaussian basis. We show the algorithm of the interface and the examples.

References

1. J. Xu, C. R. Natoli, P. Krüger, K. Hayakawa, D. Sébilleau, L. Song, K. Hatada, *Comput. Phys. Commun.* **203**, 331 (2016).
2. G. Kresse, D. Joubert, *Phys. Rev. B* **59**, 1758 (1999).
3. M.J. Frisch *et al.*, Gaussian09 Revision E.01, Gaussian Inc. Wallingford CT (2009).
4. H. Ebert *et al.*, The Munich SPR-KKR package version 7.7.0 (<http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR>) (2017).