Density-Difference-Driven Optimized Embedding Potential Method to Study the Spectroscopy of Br₂ in Water Clusters

Octavio Roncero¹

¹*Instituto de Física Fundamental (IFF-CSIC), C.S.I.C., Serrano 123, 28006, Madrid Spain.*

A variant of the density difference driven optimized embedding potential (DDDOEP) method[1] has been applied to the calculation of excited states of Br₂ within small water clusters[2]. It is found that the strong interaction of Br₂ with the lone electronic pair of the water molecules makes necessary to optimize specific embedding potentials for ground and excited electronic states, separately and using the corresponding densities. Diagnosis and convergence studies are presented with the aim of providing methods to be applied for the study of chromophores in solution. Also, some preliminary results obtained for the study of electronic states of Br₂ in clathrate cages are presented.

[1] O. Roncero, A. Zanchet, P. Villarreal, A. Aguado, *J. Chem. Phys.* , **131** , 234110 (2009)

[2] O. Roncero, A. Aguado, F. A. Batista-Romero, M. I. Bernal-Uruchurtu and R. Hernández-Lamonedá, W. Liu, *J. Chem. Theo. Comput.* **11**, 1155 (2015).