Cover Letter

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Dec. 30, 2019

Professor Tianquan (Tim) Lian
Editor-in-Chief, J. Chem. Phys.
Emory University, Atlanta, Georgia, USA

Manuscript Title: *Ab Initio Effective One-Electron Potential Operators. I. Applications for Charge-Transfer Energy in Effective Fragment Potentials*

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Dear Editor,

Here, the manuscript entitled "Ab Initio Effective One-Electron Potential Operators. I. Applications for Charge-Transfer Energy in Effective Fragment Potentials" written by B. Błasiak, Joanna D. Bednarska, Marta Chołuj and Wojciech Bartkowiak is submitted for publication in your journal, *J. Chem. Phys.* In the present work, new theoretical protocol of constructing mathematical models of extended molecular aggregates is proposed. It is based on effective one-electron potential operators (OEPs) and effective elimination of electron repulsion integrals, evaluation of which is usually a performance bottleneck in most of *ab initio* calculations. We believe that our method is general and in principle applicable to any theoretical chemistry problem that can be formulated in terms of unperturbed wavefunctions of molecular fragments. The submitted manuscript is also a development of the charge-transfer energy model in the second generation effective fragment potential (EFP2) method. Application of our OEP

method to this problem reduced calculation costs by around a factor of 20. We believe that the proposed advancement could be used in the current EFP2 model that is widely used in the scientific community working in the fields of Chemical Physics.

I hope that the submitted manuscript is suitable for publication in *The Journal of Chemical Physics*.

Sincerely yours,

Bartosz Błasiak