Cover Letter

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

Manuscript Title: *Ab Initio Effective One-Electron Potential Operators. II. Applications for Exchange-Repulsion Energy in Effective Fragment Potentials*

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Dear Editor,

Here, the manuscript entitled "Ab Initio Effective One-Electron Potential Operators. II. Applications for Exchange-Repulsion Energy in Effective Fragment Potentials" written by B. Błasiak, Robert W. Góra and Wojciech Bartkowiak is submitted for publication in your journal, *J. Chem. Phys.* In this part of a sequel "Ab Initio Effective One-Electron Potential Operators" our technique of elimination of electron repulsion integrals helped to enhance computational efficiency of the repulsive term in the EFP2 model, one of the most commonly used ab initio force field. Since repulsive EFP2 term is the second most expensive to evaluate contribution after charge-transfer term (discussed in Paper I of the submitted sequel), it is believed that our

methodological advancement will facilitate applications of the EFP2 method by reducing the computational costs when applied to condensed phase interaction energy and molecular dynamics simulations.

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

Sincerely yours,

Bartosz Błasiak