POSSIM – POlarizable Simulations with Second order Interaction Model

Version 2.0 October 2012

POSSIM is a software suite for geometry optimizations and Monte Carlo simulations with fixed-charges (OPLS-like) and polarizable (fast polarizable POSSIM and full-scale polarizable) force fields.

Selected References for the POSSIM Software:

(1) Kaminski, G. A.; Ponomarev, S. Y.; Lin. A. B. "Polarizable Simulations with Second-Order Interaction Model – Force Field and Software for Fast Polarizable Calculations: Parameters for Small Model Systems and Free Energy Calculations", *J. Chem. Theory Comput.*, *5*, 2935-2943, **2009**.

(2) Ponomarev, S. Y.; Kaminski, G. A. "Polarizable Simulations with Second-Order Interaction Model (POSSIM) Force Field: Developing Parameters for Alanine Peptides and Protein Backbone", *J. Chem. Theory Comput.*, *7*, 1415-1427, **2011**.

(3) For simulations with Fuzzy-Border continuum solvent model – Sharma, I.; Kaminski, G. A. "Calculating pKa Values for Substituted Phenols and Hydration Energies for Other Compounds with the First-Order Fuzzy-Border Continuum Solvation Model", *J. Comput. Chem.*, *33*, 2388-2399, **2012**.

Conditions for Use of the POSSIM Software:

_____ **Signature and Date**

_____ **Name**

_____ **Organization**

_____ **Address**

_____

_____ **E-mail**

If the above conditions are accepted, please sign this form and return a copy by mail to the following address:

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