Stanford

Ivan Ufimtsev

Physical Science Research Scientist

Chemistry

Bio

ACADEMIC APPOINTMENTS

- Phys Sci Res Assoc, Chemistry

Publications

PUBLICATIONS

- **Analytic first derivatives of floating occupation molecular orbital-complete active space configuration interaction on graphical processing units.** *journal of chemical physics*
  Hohenstein, E. G., Bouduban, M. E., Song, C., Luehr, N., Ufimtsev, I. S., Martínez, T. J.
  2015; 143 (1): 014111-?

- **Analytic first derivatives of floating occupation molecular orbital-complete active space configuration interaction on graphical processing units.** *journal of chemical physics*
  Hohenstein, E. G., Bouduban, M. E., Song, C., Luehr, N., Ufimtsev, I. S., Martínez, T. J.
  2015; 143 (1): 014111-?

- **An atomic orbital-based formulation of the complete active space self-consistent field method on graphical processing units.** *journal of chemical physics*
  Hohenstein, E. G., Luehr, N., Ufimtsev, I. S., Martínez, T. J.
  2015; 142 (22): 224103-?

- **An atomic orbital-based formulation of the complete active space self-consistent field method on graphical processing units** *JOURNAL OF CHEMICAL PHYSICS*
  Hohenstein, E. G., Luehr, N., Ufimtsev, I. S., Martinez, T. J.
  2015; 142 (22)

- **Generating Efficient Quantum Chemistry Codes for Novel Architectures** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Titov, A. V., Ufimtsev, I. S., Luehr, N., Martinez, T. J.
  2013; 9 (1): 213-221

- **Ab Initio Quantum Chemistry for Protein Structures** *JOURNAL OF PHYSICAL CHEMISTRY B*
  Kulik, H. J., Luehr, N., Ufimtsev, I. S., Martinez, T. J.
  2012; 116 (41): 12501-12509

- **Charge Transfer and Polarization in Solvated Proteins from Ab Initio Molecular Dynamics** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Ufimtsev, I. S., Luehr, N., Martinez, T. J.
  2011; 2 (14): 1789-1793

- **Excited-State Electronic Structure with Configuration Interaction Singles and Tamm-Dancoff Time-Dependent Density Functional Theory on Graphical Processing Units** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Isborn, C. M., Luehr, N., Ufimtsev, I. S., Martinez, T. J.
  2011; 7 (6): 1814-1823

- **Dynamic Precision for Electron Repulsion Integral Evaluation on Graphical Processing Units (GPUs)** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Luehr, N., Ufimtsev, I. S., Martinez, T. J.

2011; 7 (4): 949-954

- **GPU-accelerated molecular modeling coming of age** *JOURNAL OF MOLECULAR GRAPHICS & MODELLING*
  Stone, J. E., Hardy, D. J., Ufimtsev, I. S., Schulten, K.
  2010; 29 (2): 116-125

- **Quantum Chemistry on Graphical Processing Units. 3. Analytical Energy Gradients, Geometry Optimization, and First Principles Molecular Dynamics** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Ufimtsev, I. S., Martinez, T. J.
  2009; 5 (10): 2619-2628

- **Quantum Chemistry on Graphical Processing Units. 2. Direct Self-Consistent-Field Implementation** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Ufimtsev, I. S., Martinez, T. J.
  2009; 5 (4): 1004-1015

- **A multistate empirical valence bond model for solvation and transport simulations of OH- in aqueous solutions** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
  Ufimtsev, I. S., Kalinichev, A. G., Martinez, T. J., Kirkpatrick, R. J.
  2009; 11 (41): 9420-9430