Kaining Duanmu

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Education
University of Minnesota – Twin Cities, Ph.D. in Chemistry, 2011 – 2016
University of Science and Technology of China, B.S. in Chemical Physics, 2007 – 2011

Research
Electronic structure theories and applications
Properties of metal clusters and nanoparticles
Solid state chemistry and surface modeling
Catalysis on metal clusters and surfaces

Publications
“Partial Ionic Character Beyond the Pauling Paradigm: Metal Nanoparticles,” K. Duanmu and D. G. Truhlar, *J. Phys. Chem. C* **18**, 28069-28074 (2014). This work was highlighted in Chemical and Engineering News. http://comp.chem.umn.edu/Truhlar/docs/1046CEN.pdf
"Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals," J. L. Bao, H. S. Yu, K. Duanmu, M. Makeev, and D. G. Truhlar, *ACS Catalysis* **5**, 2070-2080 (2015).
"Atomic Oxygen Recombination at Surface Defects on Reconstructed (0001) α-Quartz exposed to Atomic and Molecular Oxygen," R. Meana-Pañeda, Y. Paukku, K. Duanmu, P. Norman, T. Schwartzentruber, and D. G. Truhlar, *J. Phys. Chem. C* **119**, 9287-9301 (2015).
"Validation of Methods for Computational Catalyst Design: Geometries, Structures, and Energies of Neutral and Charged Silver Clusters," K. Duanmu and D. G. Truhlar, *J. Phys. Chem. C* **119**, 9617-9626 (2015).
"Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters" K. Duanmu, O. Roberto-Neto, F. B. C. Machado, J. A. Hansen, J. Shen, P. Piecuch, and D. G. Truhlar, *J. Phys. Chem. C* accepted.
"Comparison of DFT to Benchmark Database for Adsorption Energies on Transition Metal Surfaces," K. Duanmu and D. G. Truhlar, submitted

Programming
“CM5PAC,” K. Duanmu, B. Wang, A. V. Marenich, C. J. Cramer, and D. G. Truhlar (2015) http://comp.chem.umn.edu/cm5pac/
“MN-VFM,” K. Duanmu, S. Luo, and D. G. Truhlar (2015) http://comp.chem.umn.edu/mn-vfm/