Publications acknowledging the Center for Simulation and Modeling

1. Z. Liu, Y. Lei, C. Gray, and G. Wang\*, “Examination of solid-solution phase formation rules for high entropy alloys from atomistic Monte Carlo simulations”, ***JOM***, (2015) DOI: 10.1007/s11837-015-1508-3.
2. S. Kattel and G. Wang, “Beneficial compressive strain for oxygen reduction on Pt (111) surface”, ***Journal of Chemical Physics***, 141 (2014) 124713.
3. S. Kattel and G. Wang, “Reaction pathway for oxygen reduction on FeN4 embedded graphene”, ***Journal of Physical Chemistry Letters***, 5 (2014) 452-456.
4. K. Liu, Y. Lei, and G. Wang, “Correlation between oxygen adsorption energy and electronic structure of transition metal macrocyclic complexes”, ***Journal of Chemical Physics***, 139 (2013) 204306.
5. H. Lv, Y. Lei, A. Datta, and G. Wang,“Influence of surface segregation on magnetic properties of FePt nanoparticles”, ***Applied Physics Letters***, 103, (2013) 132405.
6. S. Kattel and G. Wang, “A density functional theory study of oxygen reduction reaction on Me-N4 (Me=Fe, Co, or Ni) clusters between graphitic pores”, ***Journal of Materials Chemistry A***, 1 (2013) 10790-10797.
7. S. Kattel, Z. Duan, and G. Wang, “Density functional theory study of an oxygen reduction reaction on a Pt3Ti alloy electrocatalyst”, ***Journal of Physical Chemistry C***, 117 (2013) 7107-7113.
8. Z. Duan and G. Wang, “Comparison of reaction energetic for oxygen reduction reactions on Pt(100), Pt(111), Pt/Ni(100), and Pt/Ni(111) surfaces: A first-principles study”, ***Journal of Physical Chemistry C***, 117 (2013) 6284-6292.
9. X. Sang, A. Kulovits, G. Wang, and J. Wiezorek, “Validation of density functionals for transition metals and intermetallics using data from quantitative electron diffraction”, ***Journal of Chemical Physics***, 138 (2013) 084504.
10. X. Sang, A. Kulovits, G. Wang, and J. Wiezorek, “High precision electronic charge density determination for L10-ordered γ-TiAl by quantitative convergent beam electron diffraction”, ***Philosophical Magazine***, 92 (2012) 4408-4424.
11. A. Datta, Z. Duan and G. Wang, “Influence of surface segregation on the elastic property of Pt-Ni alloy nanowires”, ***Computational Materials Science***, 55, (2012) 81-84.
12. Z. Duan# and G. Wang\*, “A first principles study of oxygen reduction reaction on a Pt (111) surface modified by a subsurface transition metal M (M=Ni, Co, or Fe)”, ***Physical Chemistry Chemical Physics***, 13 (2011) 20178-20187.

Active grants using SaM Facility

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| Project Title | Atomistic simulation investigation on processing-structure-property relation of magnetic metal alloy nanostructures |
| Agency | National Science Foundation |
| PI | Prof. G.F. Wang |
| Co-PI | None |
| Place of Research | University of Pittsburgh |
| Amount | $ 300,000 |
| Project Period | 9/1/2014-8/31/2017 |
| Description | In this project, we will predictively model the surface segregation, atomic ordering, and magnetic behavior of the metallic alloy nanostructures with diameter up to 10 nm and further elucidate the inter-relation of their processing, structure, and magnetic property using the first-principles based computational methods. |