Materials List for:

Multiscale Sampling of a Heterogeneous Water/Metal Catalyst Interface using Density Functional Theory and Force-Field Molecular Dynamics

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Materials

Name	Company	Catalog Number	Comments
VASP software	Computational Materials Physics, Dept. of Physics, University of Vienna	vasp.5.4.4	Standard parallel VASP executable in the newest version.
LAMMPS software	Sandia National Laboratory	31Mar17-dp	Double-precision, parallel LAMMPS executable from 31 March 2017.
VMD software	Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign	1.9.3	Standard VMD executable in the newest version.
MCPliQ software	Getman Research Group, Dept. of Chemical and Biomolecular Engineering, Clemson University		Executable and input files for the MCPliQ software availabe from the Getman Research Group GitHub page.
JoVE article scripts	Getman Research Group, Dept. of Chemical and Biomolecular Engineering, Clemson University		Python scripts for this JoVE manuscript available from the Getman Research Group GitHub page.
H2O PDB file	Getman Research Group, Dept. of Chemical and Biomolecular Engineering, Clemson University or RCSB Protein Data Bank		PDB file for a water molecule, available from the Getman Research Group GitHub page or at http://www.rcsb.org/ligand/HOH.