Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Structural characterizations of water-metal interfaces with large-scale first principles molecular dynamics[1] KEVIN RYCZKO, University of Ontario Institute of Technology, ISAAC TAMBLYN, National Research Council of Canada / University of Ontario Institute of Technology — We analyze and compare the structural, dynamical, and electronic properties of liquid water next to prototypical metals including Pt, graphite, and graphene. Our analysis is built on Born-Oppenheimer molecular dynamics (BOMD) generated using density functional theory (DFT). All calculations we present use large simulation cells, allowing for an accurate treatment of the water-electrode interfaces. We have included van der Waals (vdW) interactions through the use of the optB86b-vdW exchange correlation functional, as it includes non-local interactions and has shown to give good results with respect to structural experiments. Comparisons with the Perdew-Burke-Ernzerhof (PBE) exchange correlation functional are also shown. We find an initial peak, due to chemisorption, in the density profile of the liquid water-Pt interface not seen in the liquid water-graphite interface, liquid water-graphene interface, nor interfaces covered in other literature. To further investigate this chemisorption peak we also report differences between single water adsorption on the Pt and graphite surfaces. In total, over 135 ps of BOMD data was generated and analyzed.

[1]The authors acknowledge NSERC, SOSCIP and Compute Canada for funding and com- putational resources.

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Date submitted: 09 Nov 2016 Electronic form version 1.4