Towards accurate prediction of catalytic activity in IrO_2 nanoclusters via first principles-based variable charge force field

Fatih G. Sen,[1] Alper Kinaci,[1] Badri Narayanan,[1] Stephen K. Gray,[1,3] Michael J. Davis,[2] Subramanian K.R.S. Sankaranarayanan,[1,3] Maria K.Y. Chan[1,3]

[1]Center for Nanoscale Materials, Argonne National Laboratory, 9700 S. Cass Ave., Lemont, IL 60439 USA
[2]Chemical Sciences Division, Argonne National Laboratory, 9700 S. Cass Ave., Lemont, IL 60439 USA
[3]Computation Institute, the University of Chicago, 5735 S. Ellis Ave., Chicago, IL 60637 USA

Supporting Information

Supporting information 1 - Vibrational properties of rutile IrO_2

Vibrational properties give information about the elastic stability, thermal stability, thermal conductivity and electrical conductivity. We test if the MS-Q force field we developed is capable of predicting these properties for IrO_2. Figure S1 displays the calculated phonon dispersions of IrO_2, along high symmetry directions in the reciprocal space, calculated with MS-Q and DFT. It should be noted that the phonon frequencies are not a part of the training set. Figure S1 indicates that the dispersion curves below 10 THz show good agreement with the DFT results. Phonon frequencies higher than 10 THz do not match with DFT results as well as low frequency modes. However, high frequency modes are not predominant carriers of thermal currents due to their smaller mean free paths.[1] Consequently, we can expect that the MS-Q FF we developed should be able to describe thermodynamic, thermal, and elastic behaviors at low temperature, although experimental information and further testing is necessary to ascertain the accuracy.

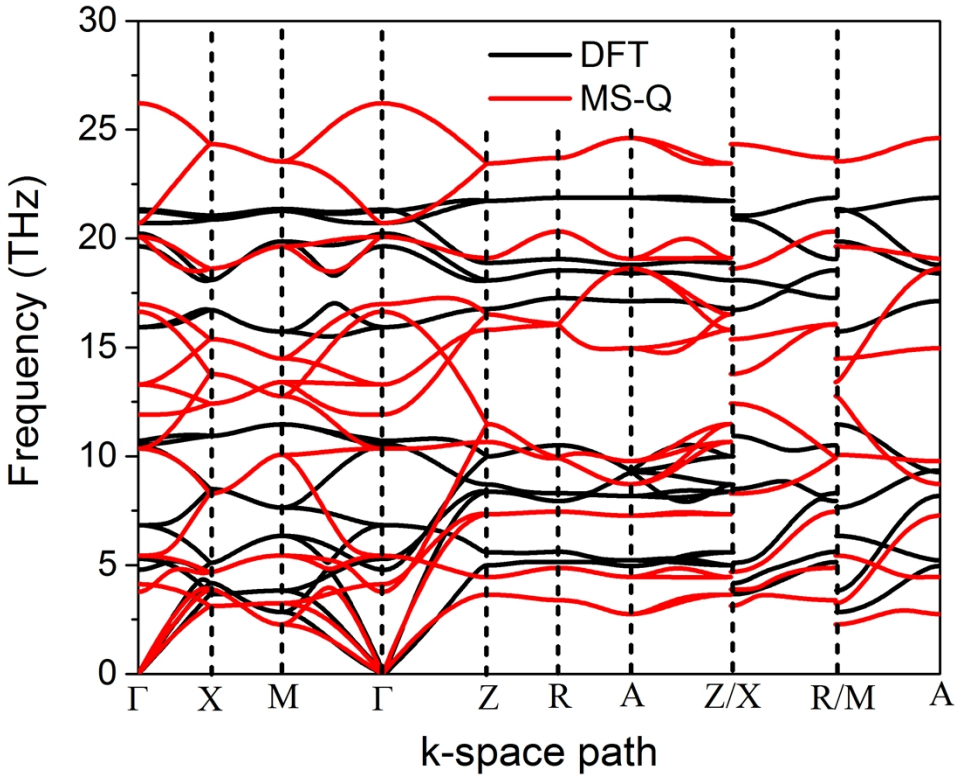

Figure S1. Phonon dispersion of rutile IrO_2 calculated with MS-Q along the high-symmetry reciprocal space points (red) and compared to DFT results (black).

References

1. Sevik, C.; Kinaci, A.; Haskins, J. B.; Cagin, T., *Physical Review B* **2011,** *84* (8).