Abstract Submitted
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Structure, Spectroscopy and Thermodynamics at the Water – Graphene Interface[1] TOD PASCAL, The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, CRAIG SCHWARTZ, Stanford Synchrotron Radiation Laboratory, Menlo Park, CA 94025, USA, KEITH LAWLER, Department of Chemistry, University of Nevada Las Vegas, Las Vegas, NV 89154, USA, DAVID PRENDERGAST[2], The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — The recent discovery of an ordered two-dimensional phase of water with a square lattice between graphene sheets has led to tremendous interest in the structure of confined water, particularly under pressure.[1] Despite being recently discovered, this finding is fiercely being debated, with other researchers suggesting that the observed structures is due to the presence of NaCl, while various theoretical models predict the formation of water ice between graphene only under enormous external pressures.[1-3] Herein, by examining the EELS data, combined with simulated spectroscopy calculations and molecular dynamic simulations, we examine the thermodynamic properties of nano-encapsulated water, and demonstrate how charge transfer and chemical defects alters the phase diagram. [4]

1. Algara-Siller, G. et al., Nature 519, 443–445 (2015).

2. Mario, S. F., Neek-Amal, M. & Peeters, F. M., arXiv:1509.08242 [cond-mat] (2015)

3. Jiao, S. & Xu, Z., arXiv:1509.07215 [cond-mat] (2015)

4. Schwartz, C. et al., In preparation

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