Abstract Submitted
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Viscosity of ultrathin water films confined between oxide surfaces – ab initio and classical molecular dynamics simulations[1] PETER J. FEIBELMAN, GARY S. GREST, Sandia National Laboratories, NEIL HARIA, CHRISTIAN D. LORENZ, King's College London — We compare estimates based on ab initio (DFT/PBE) and on classical molecular dynamics simulations of the viscosity of 2, 3 and 5-layer water films confined between hydrophilic kaolinite surfaces. Results were obtained by constraining the confining surfaces to move in +x and -x directions at equal speeds of 1-200 m/sec and loads up to 1 GPa. In neither simulation approach did the calculated viscosity of the confined water exceed that of bulk water by more than an order of magnitude. Thus neither supports the idea that nano-confinement dramatically enhances water's viscosity.

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