Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Confined water between two graphene layers FRANCOIS PEETERS, MARIO SOBRINO FERNANDEZ, MEHDI NEEK-AMAL, University of Antwerp, Dept. of Physics, 2020 Antwerp, CONDENSED MATTER THEORY TEAM — Water confined between two layers with a separation of a few Angstrom forms a layered two- dimensional ice structure. Using large scale molecular dynamics simulations with the adoptable ReaxFF interatomic potential we found that monolayer ice with a rhombic-square structure nucleates between graphene layers which is non-polar and non-ferroelectric. We provide different energetic considerations and H-bonding results that explain the inter-layer and intra-layer properties of two-dimensional ice. The controversional AA-stacking found experimentally [G. Algara-Siller et al. Nature 519, 443445 (2015)] is consistent with our minimum energy crystal structure of bilayer ice. Furthermore, we predict that odd-number of layers of ice has the same lattice structure as monolayer ice, while even number of ice layers exhibit the square ice AA-stacking of bilayer ice.We predict that an in-plane electric field polarizes the water molecules resulting in distinct-ferroelectricity. Electrical hysteresis in the response of the total dipole moment of monolayer ice is found

Francois Peeters
University of Antwerp, Dept. of Physics, 2020 Antwerp

Date submitted: 06 Nov 2015 Electronic form version 1.4