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Hydrogen bond network ordering of liquid water confined between two metallic plates studied by *ab initio* molecular dynamics MARIVI FERNANDEZ-SERRA, Physics & Astronomy SUNY, Stony Brook — We present an *ab initio* molecular dynamics study of liquid water confined between two palladium $\langle 111 \rangle$ surface slabs, at room temperature. We analyze in detail the layering and ice-Ih-type ordering of water molecules close to the metal interfaces. In particular we show how water molecules next to the metal surface display a very different structural and dynamic behavior as compared those in the “bulk” regions, which can be easily characterized using infra-red spectroscopy. Hydrogen bonds near the metallic interfaces are strengthened, inducing a characteristic ordering which decays with de distance from the surfaces. Our preliminary results show that this confined water presents an asymmetrical and stable structure as a function of Z (axis perpendicular to the surfaces) which results in a characteristic system with an overall ordering of the water molecules resembling that of ferroelectric systems.

Marivi Fernandez-Serra
Physics & Astronomy SUNY, Stony Brook

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