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Quasicrystal and ice phases tiled with pentagons in confined water

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Bulk water is known to form a wealth of ice polymorphs and two distinct amorphous phases. Less is known of the structures that confined and interfacial water can adopt, and whether there is a correspondence between the structures and phase diagrams of water in bulk and in confinement. In this talk I will present a molecular simulations study of the phase behavior of a water bilayer confined between two non-hydrogen bonding walls and demonstrate that a water bilayer also presents rich polymorphism, including an ice crystal fully tiled by pentagons and a quasicrystal, the first ever reported for water. The water quasicrystal and the ice polymorph tiled with pentagons are not templated by the confining surfaces. This indicates that these novel phases are intrinsically favored in bilayer water and suggests that they may be formed, without confinement, on surfaces.

[1] J.C. Johnston, N. Kastelowitz and V. Molinero, "Liquid to quasicrystal transition in bilayer water," J. Chem. Phys. 133, 154516 (2010)
[2] N. Kastelowitz, J. C. Johnston and V. Molinero, "The anomalously high melting temperature of bilayer ice," J. Chem. Phys. 132, 124511 (2010).