Abstract Submitted
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**A computational DFT study of structural transitions in textured solid-fluid interfaces**[1] PETR YATSYSHIN, Department of Chemical Engineering, Imperial College London, London, UK, ANDREW O. PARRY, Department of Mathematics, Imperial College London, London, UK, SERAFIM KALLIADASIS, Department of Chemical Engineering, Imperial College London, London, UK —
Fluids adsorbed at walls, in capillary pores and slits, and in more exotic, sculpted geometries such as grooves and wedges can exhibit many new phase transitions, including wetting, pre-wetting, capillary-condensation and filling, compared to their bulk counterparts. As well as being of fundamental interest to the modern statistical mechanical theory of inhomogeneous fluids, these are also relevant to nanofluidics, chemical- and bioengineering. In this talk we will show using a microscopic Density Functional Theory (DFT) for fluids how novel, continuous, interfacial transitions associated with the first-order prewetting line, can occur on steps, in grooves and in wedges, that are sensitive to both the range of the intermolecular forces and interfacial fluctuation effects. These transitions compete with wetting, filling and condensation producing very rich phase diagrams even for relatively simple geometries. We will also discuss practical aspects of DFT calculations, and demonstrate how this statistical-mechanical framework is capable of yielding complex fluid structure, interfacial tensions, and regions of thermodynamic stability of various fluid configurations. As a side note, this demonstrates that DFT is an excellent tool for the investigations of complex multiphase systems.

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Petr Yatsyshin
Imperial College London

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