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## Water at the interface between defective graphene and Cu or Pt (111) surface

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The presence of defects in the graphenic layers deposited on metal surfaces modifies the nature of the interaction. Unsaturated carbon atoms, due to vacancies in the lattice, form strong organometallic bonds with surface metal atoms that highly enhance the binding energy between the two materials. We investigate by means of a wide set of dispersion-corrected density functional theory calculations how such strong chemical bonds affect both the electronic properties of these hybrid interfaces and the chemical reactivity with water, which is commonly present in the working conditions. We compare different metal substrates (Cu vs. Pt) that present a different type of interaction with graphene and with defective graphene. This comparative analysis allows us to unravel the controlling factors of water reactivity, the role played by the carbon vacancies and by the confinement or “graphene cover effect”. Water is capable of breaking the C-Cu bond by dissociating at the undercoordinated carbon atom of the vacancy, restoring the weak van der Waals type of interaction between the two materials that allows for an easy detachment of graphene from the metal, but the same is not true in the case of Pt, where C-Pt bonds are much stronger. These conclusions can be used to rationalize water reactivity at other defective graphene/metal interfaces.

### Biography

Daniele Perilli obtained his MSc in Chemistry in 2017 at the University of Milano-Bicocca with a thesis on the computational study of defective graphenic systems supported on metals. His work of bachelor and master thesis has been included in three international peer-reviewed articles. He is now pursuing his PhD degree in Materials Science under the supervision of Prof. Cristiana Di Valentin. His current research focuses on quantum mechanical simulations of low dimensional materials, in particular electronic structure and catalysis of metal supported and defective h-BN sheet.

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