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Her research has mostly focused on the study of the electronic and transport properties of materials, and the modification of their electronic properties by defects, molecular adsorption, or interaction with substrates, by means of atomistic (Density Functional Theory and tight-binding) and quantum transport (NEGF) simulation tools. More recently, she has started working on classical Molecular Dynamics and hybrid (QM/MM) simulations of biomolecules. She has co-authored over 35 peer-reviewed publications in high-impact international journals, which have received more than 1800 citations