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Adsorbates at periodic metal and insulating surfaces: From structure to non-equilibrium dynamics

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The theoretical modelling of atoms and molecules adsorbed at solid surfaces is key to the understanding of important physicochemical phenomena and applications, ranging from heterogeneous catalysis over surface femtochemistry and electrochemistry to astrochemistry, to name just a few. In this talk, I will review some of our work over the last decades on the structure, spectroscopy, and – mostly photoinduced – dynamics, of adsorbates at periodic metal and insulating surfaces. Underlying methods will be covered "on the fly". Specific examples include quantum size effects in thin metal films [1,2], femtosecond-laser driven, "hot-electron" mediated dynamics and reactions at metal surfaces [3,4,5], and, finally, the vibrational spectroscopy, dynamics and kinetics of small molecules at insulator surfaces, notably for CO on NaCl [6,7,8].

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