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Kinetic Monte Carlo studies of the behavior of CO on sulfur-covered Pd(100) surface DOMINIC ALFONSO, National Energy Technology Laboratory — Investigations of the behavior of CO on the surface of Pd modified with sulfur were carried out using first-principles Kinetic Monte Carlo method. In particular, the influence of adsorbed sulfur on the adsorption, diffusion and desorption of CO on the Pd(100) surface was studied. A kinetic Monte Carlo code was developed which enables the simulation of hosts of competing elementary steps with lateral interaction between the adspecies taken into account. The barriers and energetics of the relevant elementary processes were determined by density-functional theory. The rates entering the simulation were derived using transition state theory. The adsorbates were assumed to interact via pairwise additive interactions. We demonstrate that adsorbed sulfur has an adverse effect on the behavior of CO on Pd(100).

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