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Reactive properties of chemically modified Pd(100) surface revealed by Kinetic Monte Carlo simulations DOMINIC ALFONSO, National Energy Technology Laboratory — The interaction of H_2 and CO with sulfur-covered Pd(100) surface represents a prototype model for understanding the various reasons for the poisoning of palladium by sulfur compounds. The use of Kinetic Monte Carlo method to investigate this system was explored. A Kinetic Monte Carlo code was developed and used to monitor the hosts of competing elementary steps associated with the adsorption, diffusion and desorption of H_2 and CO on the metal surface. The input parameters such as rate of reactions and lateral interactions were obtained from density functional theory calculations within the generalized gradient approximation. We demonstrate that Kinetic Monte Carlo simulation is a powerful tool for elucidating the microscopic details of the behavior of H_2 and CO on the poisoned surface.

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