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Role of hydrogen on catalytic reduction of nitric oxide on selected transition metal surfaces FAISAL MEHMOOD, ANAND U. NILEKAR, MANOS MAVRIKAKIS, University of Wisconsin-Madison — Self-consistent periodic DFT-GGA calculations are used to investigate the NO reduction reaction in presence of atomic H on seven close-packed transition metal surfaces namely, Cu(111), Ag(111), Pd(111), Pt(111), Rh(111), Ir(111), and Ru(0001). The chemisorption of atomic (N, O, H) and molecular (NO, NH, OH, HNO, NOH, HNOH, H_2NO) reaction intermediates has been systematically studied on each metal surface and the preferred sites and binding energies are determined for a 1/4 ML surface coverage. The activation energy barriers for the relevant set of reactions have also been calculated. Based on these results, the potential energy surfaces (PESs) for direct and H-assisted NO reduction reaction on all the metal surfaces have been constructed. These PESs are used for elucidating the trends for various elementary steps involved in the NO reduction reaction, across the periodic table. These PESs indicate that on (111) surfaces of Cu, Ag, Pd and Pt, H assisted NO reduction is quite favorable by either NOH or HNO reaction intermediate. For remaining three close-packed metal surfaces, i.e. Rh, Ir and Ru we do not find significant change due to presence of H. We also find that the presence of extra H may contribute in formation of HNOH or H_2NO on the surface that cause barrier to reduce even further.

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