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Ab-initio Density Functional Theory Based Study of Adsorption of No on Pt, Pd and Ir Surfaces[1] CHURNA BHANDARI, University of Texas El Paso — Among many chemical by-products released from combustion engines and other industrial processes, NO is one of the most harmful components which causes significant pollution to the environment. To minimize this effect and produce pollutionless energy, one needs an efficient catalyst which can change it into some other harmless forms. To study the catalytic behavior of metals, a powerful tool so called DFT is implemented. In this talk, I will mainly discuss the adsorption behavior of NO on the clean Pt, Pd and Ir surfaces studied on the basis of time independent DFT calculation.

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