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Predictive Modeling of Metal-Organic Chains with Active Metal Site NASEEM UD DIN, DUY LE, TALAT RAHMAN, Univ of Central Florida — Creation, stabilization, characterization and control of single atom transition metal (TM) sites may lead to significant advancement of the next-generation catalyst. Motivated by the experimental results of Skomski et al. [1], we have performed density functional theory based calculations of TM-dipyridyltetrazine (DT) chains in which TM atoms are stabilized and separated by the DT molecules. Our calculations show that the formation energies of the chains are high, suggesting that these chains can easily be synthesized and stabilized. Moreover, by calculating the adsorption energies of CO, O_2 and O atom on the metal atom sites of the chains we found that these molecules/atoms strongly bond to TM atoms Mo, Cr, Fe and Co occupying these sites, suggesting that these TM-DT chains are potential candidates for CO oxidation catalyst. Details of reaction pathway (energetic and kinetic) of CO oxidation on the chains will be also presented and discussed. [1] D. Skomski, C.D. Tempas, K.A. Smith, and S.L. Tait, "Redox-Active On-Surface Assembly of Organic Chains with Single-Site Pt(II)," Journal of the American Chemical Society **136**, 9862-9865 (2014).

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