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Catalytic Reactions of DNT and TNT Molecules on Porphyrin Complexes KEITH WARNICK, BIN WANG, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory — Reactions of molecules with substrates can be used to identify them, as in sensor applications. Here we examine reactions of DNT and TNT molecules on porphyrin and metal-porphyrin via first-principles DFT calculations. We find that the oxidation of DNT by O₂ using Fe-porphyrin as a catalyst is exothermic. The affinity of O₂ to Fe-porphyrin weakens the O₂ intramolecular bond, which lowers the oxidation reaction barrier is lowered by ~ 1 eV. Substrate effects on this process are accounted for. One way to use this selective oxidation reaction for DNT/TNT sensor applications is to exploit the metal-semiconductor transition in thin-film VO₂ to detect the energy deposited by the exothermic reaction between the adsorbed molecules. This work was supported in part by DTRA grant HDTRA1-10-0047.

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