Abstract Submitted
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Room-temperature self-cleaning molecular sensing by catalytic reactions[1] KEITH H. WARNICK, BIN WANG, Dept. of Phys. and Astr., Vanderbilt University, DAVID E. CLIFFEL, DAVID W. WRIGHT, Dept. of Chem., Vanderbilt University, RICHARD F. HAGLUND, SOKRATES T. PANTELIDES, Dept. of Phys. and Astr., Vanderbilt University — New sensing techniques using self-cleaning nanosensors for molecular detection are in demand. Here we describe a room-temperature process in which a nanostructured substrate catalyzes the reaction of a target molecule with atmospheric oxygen and the reaction energy is absorbed by the substrate, where it can in principle be detected. Specifically, we report first-principles calculations describing a reaction catalyzed by Fe-porphyrin at room temperature that breaks O_2, incorporates an oxygen into the methyl group of 2,4-dinitrotoluene (DNT) and releases 1.9 eV per reaction. The atomic oxygen left on the Fe site can be removed by reacting with another DNT molecule, making the whole process self-cleaning. The reaction energy absorbed by the substrate can in principle be detected optically, as for example, by detecting the metal-insulator phase transition in VO_2. We further explore issues of sensitivity and selectivity in exploiting this reaction for solid-state molecular sensing.

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