491b A Photocatalytic Study of Ets-10 for the Oxidation of Organic Compounds

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In recent years, the use of semiconductors as photocatalysts has gained interest due to their unique potential applications and their ability to promote reactions at low temperatures. However, many of these semiconductor materials have significant disadvantages that prevent them for being used widely in industry, such as a high energy band gap and a structure that prevents a high quantum yield (reaction rate/number of photons absorbed). Here, the microporous titanium silicate ETS-10 is investigated, since its unique structure may allow for a fundamental understanding of the material and surface properties needed overcome some of the disadvantages of traditional semiconductors like anatase. ETS-10 is a microporous titanosilicate discovered by Kuznicki (US Pat. 4853202) and is composed of octahedral chains of TiO_6 connected to tetrahedral SiO_4. These chains then stack perpendicular to each other to form a 7.5 Å, three-dimensional channel structure with a stoichiometry of $(Na, K)_2TiSi_5O_{13}$.. These TiO_6 chains, which are insulated by the SiO_4 groups, form a “quantum wire” for the formation electron-hole pairs upon irradiation with UV photons. ETS-10 has be studied using an array of experimental and computational methods, such as an in-situ DRIFT cell, UV/vis diffuse reflectance, XRD, N_2 adsorption, and DFT calculations, to accomplish two main objectives. First to optimize the ETS-10 structure in order to lower the band gap energy. Advances in area have been achieved by the use of transition metals such as V, Cr, Fe, and Nb, which substitutes for the Ti atoms in the chain. The second has been to use in-situ DRIFT measurements to develop reaction mechanisms for the decomposition of methanol, ethene, and ethanol in the presence of ETS-10 and compare them to the already published studies on TiO_2. All of these measurements will be closely tied to molecular modeling efforts that will be used to guide experiments and help explain the experimental results.