

Cover Picture

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The cover picture illustrates how water affects the UV/Vis spectra of titanium zeolites. Tetrahedral titanium sites show a characteristic band (blue), not present in all-silica zeolites spectra (black), caused by a ligand-to-metal charge transfer process (LMCT) involving p-orbitals of framework oxygens and the empty d-orbitals localized on Ti (yellow arrow). The band is red-shifted when, due to water adsorption, titanium becomes penta- (green) or hexa-coordinated (red). In their article on page 538, Fois et al. highlight the microscopic details of the water-induced bathochromism by simulating electronic spectra of Ti-zeolites via a periodic DFT approach.

