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## Quantum chemistry aided FTIR spectroscopy to distinguish internal and external Brønsted acidic sites of zeolite nano-crystals

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Microporous nano-crystals of zeolites are key ingredients in more than 50% of heterogeneous catalysts, which contribute to manufacturing the majority of chemical products. Their Brønsted acidic hydroxyl groups (BA-OH) play pivotal role in many reactions. The presence of BA-OH sites on the crystallite surface bears of special interest, due to diffusion limitations inside of their micropores. Yet distinction of the internal and external BA-OH sites has been ambiguous. Here we show that clear distinction can be made by Fourier Transform Infrared (FTIR) spectroscopy when both diffuse reflectance (DR) and transmission (TR) sampling techniques are employed. Different laboratories use these techniques interchangeably for characterizing solids. To our surprise, we observed very different BA-OH spectra on some zeolites when measured by these two methods. Since physical and chemical differences do not generate such large spectral deviations, we conjectured that emphasized vibrational intensities of the surface and bulk BA-OH groups cause the differences when DR or TR technique is used, respectively. To prove our point we performed selective pyridine adsorption experiments on Chabazite (H-CHA) and H-SAPO-34 zeolites and also computed the density functional theory (DFT) based FTIR spectra of their four geometrically different BA-OH groups in the bulk and on the surface, which confirmed the conjectured vibrational differences. These zeolites are key ingredients of new catalysts for diesel-automobile exhaust control and for the methanol to olefin, MTO, technology.

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## Direct-writing of paper based conductive track using silver nano-ink for electrochemical application

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To the best of our knowledge, to date there is no report for the synthesis of silver nanoparticles capped with oleylamine (AgNPs/OLA) and then use of NPs in the preparation of paper based conductive track for electroanalytical application. The synthesized OLA capped AgNPs was characterized with TEM, UV-visible, EDX, FTIR and TGA to know the size, composition and surface modification of NPs. The best electrical conductivity of printed electronic ( $0.11 \times 10^5 \text{ S cm}^{-1}$ ) was obtained by applying a 10% AgNPs nano-ink solution on photo paper while keeping sintering temperature at 150°C for 60 min of sintering time. A conductive nano-ink was used to prepare electrodes (counter, reference and working) on photo paper and utilized in cyclic voltammetry (CV) measurement. In addition, we demonstrated the lighting of LED when conductive track was connected to a 1.5 V battery. The advantages of this paper-based flexible electrodes are user-friendly, cost effective and multiple analyses (> 50 times) in CV compared to other printed electrodes.

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