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NEW DESCRIPTORS TO CHARACTERIZE POROUS MATERIALS

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The potential use of nanoporous solids for CO_2 capture explains the huge academic effort devoted to the synthesis and evaluation of novel materials, however, the traditional trial-and-error research method are prohibitive in view of the task in hand. While the chemoinformatics has been intensively employed in the pharmaceutical and chemical research industries, only a handful attempts have been reported so far on the adsorption in porous solids [1-3]. A complete lack of "descriptors" able to precisely characterize key features of crystalline porous materials (confinement, periodicity, surface chemistry, etc.) may explain this situation. In this work we present a series of new descriptors which can be classified as topological (surface distribution of local curvature-H_A), and energetic/electronic (electrostatic-potential energy surface distribution-σ_e, local electrostatic-potential gradient distribution-$\nabla\sigma_e$). The aforementioned descriptors have been computed using adapted force fields and *ab initio* calculations, and applied to characterize a database of 20 different Metal Organic Frameworks (MOF) solids involving different functionalized imidazolate organic linkers [3]. The comparison of H_A and σ_e profiles for two Zn-based Zeolitic Imidazolate Frameworks (ZIF) is shown in Figure 1

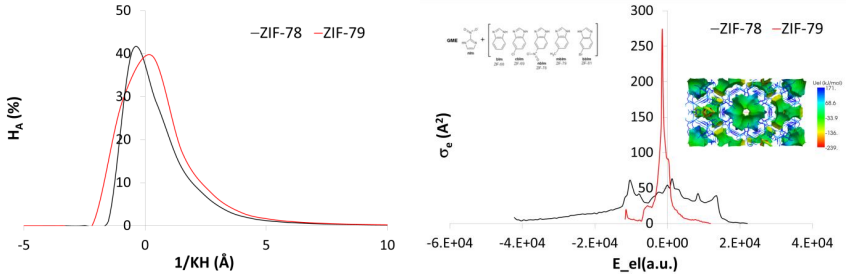

Fig. 1. Comparison H_A (left) and σ_e (right) profiles of ZIF-78 (nitro group) and ZIF-79 (methyl group). 1/KH represents the inverse of local curvature, and E_el is the local electrostatic potential energy.

While both solids have similar topology and confinement (H_A) their polar nature (σ_e) is very different (reflected by their different hydrophobicity [3]). Preliminary results to construct quantitative structure property relationships (QSPR) based models show that these descriptors are able to recover some natural properties like the porosity ratio, the global mean curvature, and the polar nature of the solids.

1. Wu D. et al. *Langmuir*, 2012, **28:** 12094.
2. Kim D. et al. *Cat. Today*, 2007, **120**: 317.
3. Amrouche H. et al. *RSC Adv.*, 2012, **2:** 6028.

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