Spatial Analysis of Crystallographically Controlled Voids in Porous Crystalline Porphyrins

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The geometric features of voids in porous materials have a large effect on properties such as molecular transport, adsorption, catalytic activity, and host/guest interactions of other types. Porphyrin hosts, although they are molecular crystals, offer relatively good thermal and chemical stability, in addition to being intrinsically semiconductive at the molecular level. In this paper, we describe our progress in the search for candidate porphyrinic structures with the required porosity for selected functional materials applications. Computational geometric characterization techniques are applied to estimate the surface area, porosity, pore volume, and local pore sizes from deposited crystallographic information, allowing for synthesis-free estimation of material performance characteristics.