Novel topologies of zinc imidazolate ($ZnIm_2$) prepared by mechanochemistry

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Metal-organic frameworks (MOFs) are highly porous, crystalline materials composed of metal nodes and organic linkers, known for their extremely large surface area and ability to tailor their structure. An interesting subclass of MOFs are zeolitic imidazolate frameworks (ZIFs). [1] The archetypal example of the ZIF materials family, zinc imidazolate ($ZnIm_2$), has been studied due to its remarkable topological diversity. To date, at least 24 crystallographically-distinct forms in 19 topologies have been documented. [2] The synthesis of these diverse topologies is mainly achieved *via* solvothermal methods, often resulting in (pseudo)polymorphic mixtures. A more sustainable approach, mechanochemical synthesis, has emerged as a promising alternative for exhaustive polymorph screening, using structure-directing effects of different liquids and salts. [3,4]

In this study, we introduce new solid forms of $ZnIm_2$, synthesized by mechanochemistry *via* the use of different solid and liquid templates and pore-filling agents. Comprehensive experimental characterization—including PXRD, IR, SEM, and EPR—alongside rigorous computational exploration utilizing molecular dynamics (MD) and dispersion-corrected periodic density functional theory (DFT) calculations, substantiate our findings.

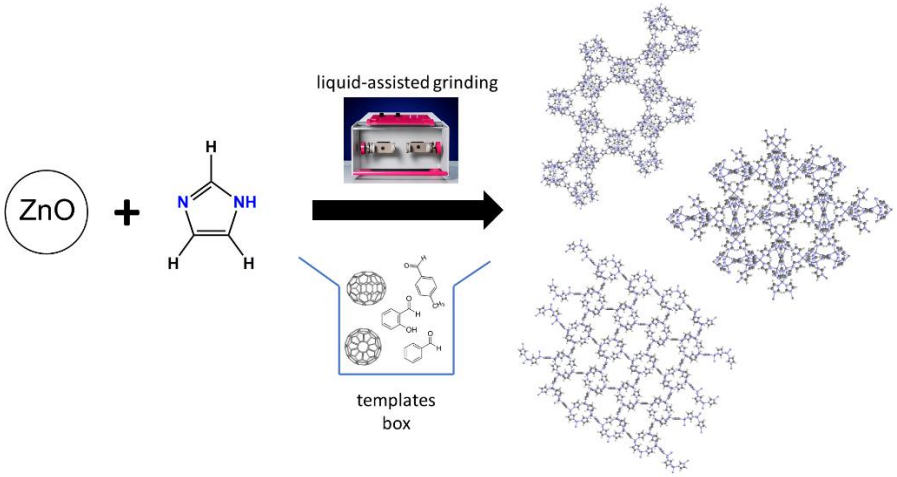


Figure 1. *Scheme of mechanochemical synthesis of new $ZnIm_2$ topologies*

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