Amorphous zeolitic imidazolate frameworks with D_{4h} local symmetry

Phillip M. Maffettone, Jerome Luchesa-Smith, Andrew B. Cairns, Matthew G. Tucker, David Keen, Leigh Connor, Mark Wilson, and Andrew L. Goodwin

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Abstract

While metal-organic frameworks (MOFs) have remained a subject of intense study, there has been a recent surge in interest regarding disordered states in these frameworks, including amorphous and liquid phases. In tandem, zeolitic imidazolate frameworks have been pursued as MOF analogues to inorganic zeolites. Here we present an amorphous zeolitic imidazolate framework composed of palladium metal centers. Due to the unique square-planar coordination geometry, previous approaches to analyzing amorphous MOF structures are incommensurate with the observed total scattering data. We develop a square-planar, continuous random network model, which can explain the distinct total scattering observed in this material. The result not only presents a new opportunity for materials design, but a vindication of the discretionary power of the total scattering pattern.