Supporting Information

for

Mechanical Properties and Nanostructure of Monolithic Zeolitic Imidazolate Frameworks: A Nanoindentation, Nanospectroscopy and Finite-Element Study

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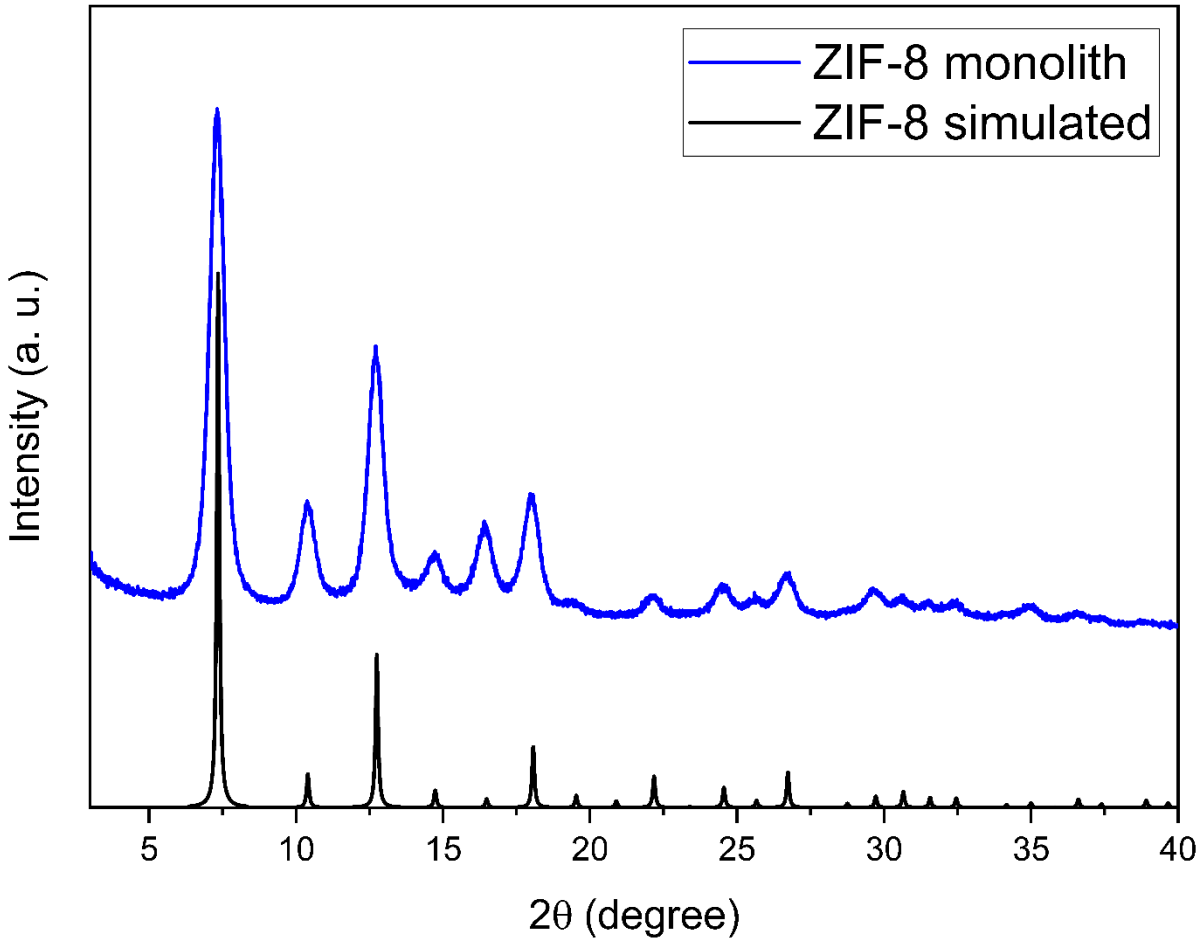

Figure S1. XRD pattern of ZIF-8 monolith in comparison with the simulated pattern from the Cambridge Structural Database (CCDC code: TUDKEJ).

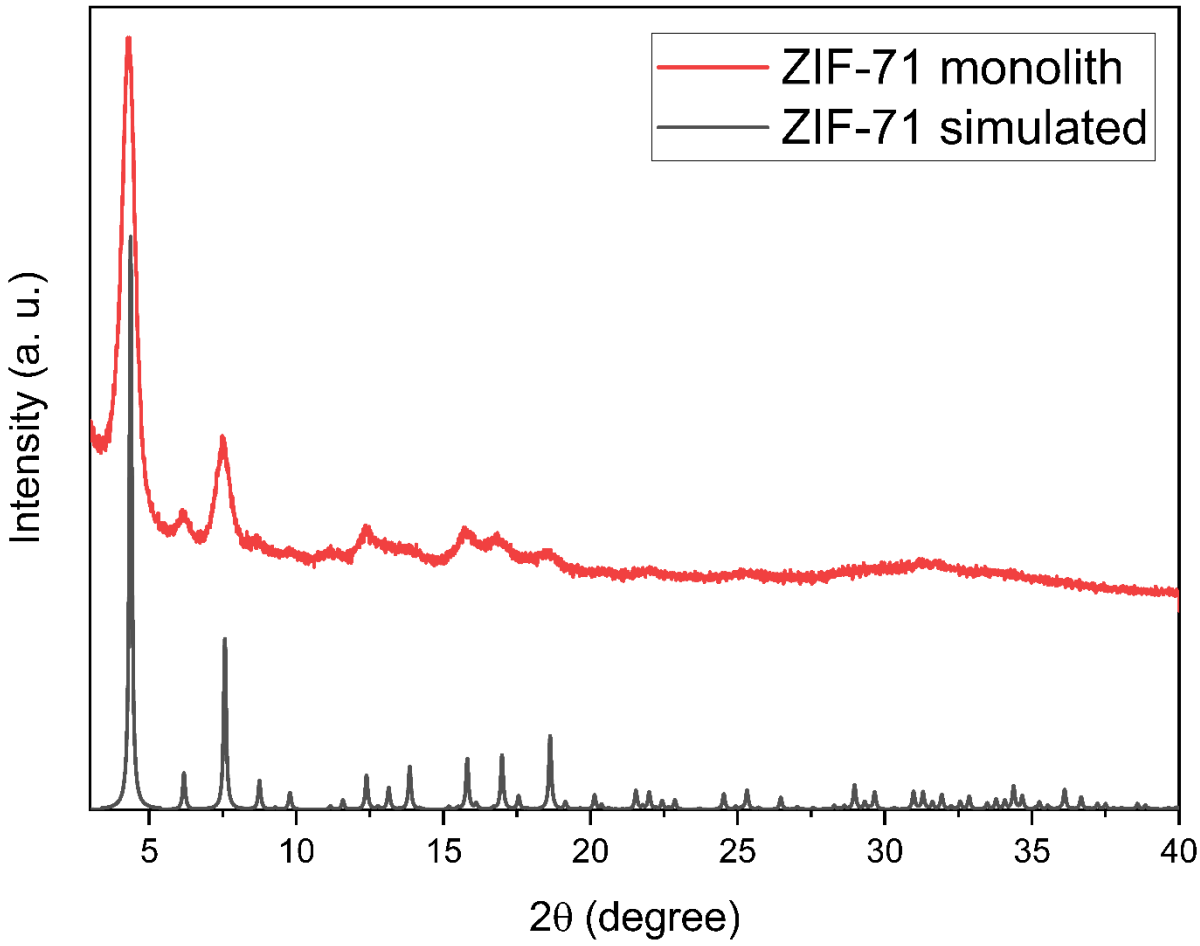

Figure S2. XRD pattern of ZIF-71 monolith in comparison with the simulated pattern from the Cambridge Structural Database (CCDC code: GITVIP).

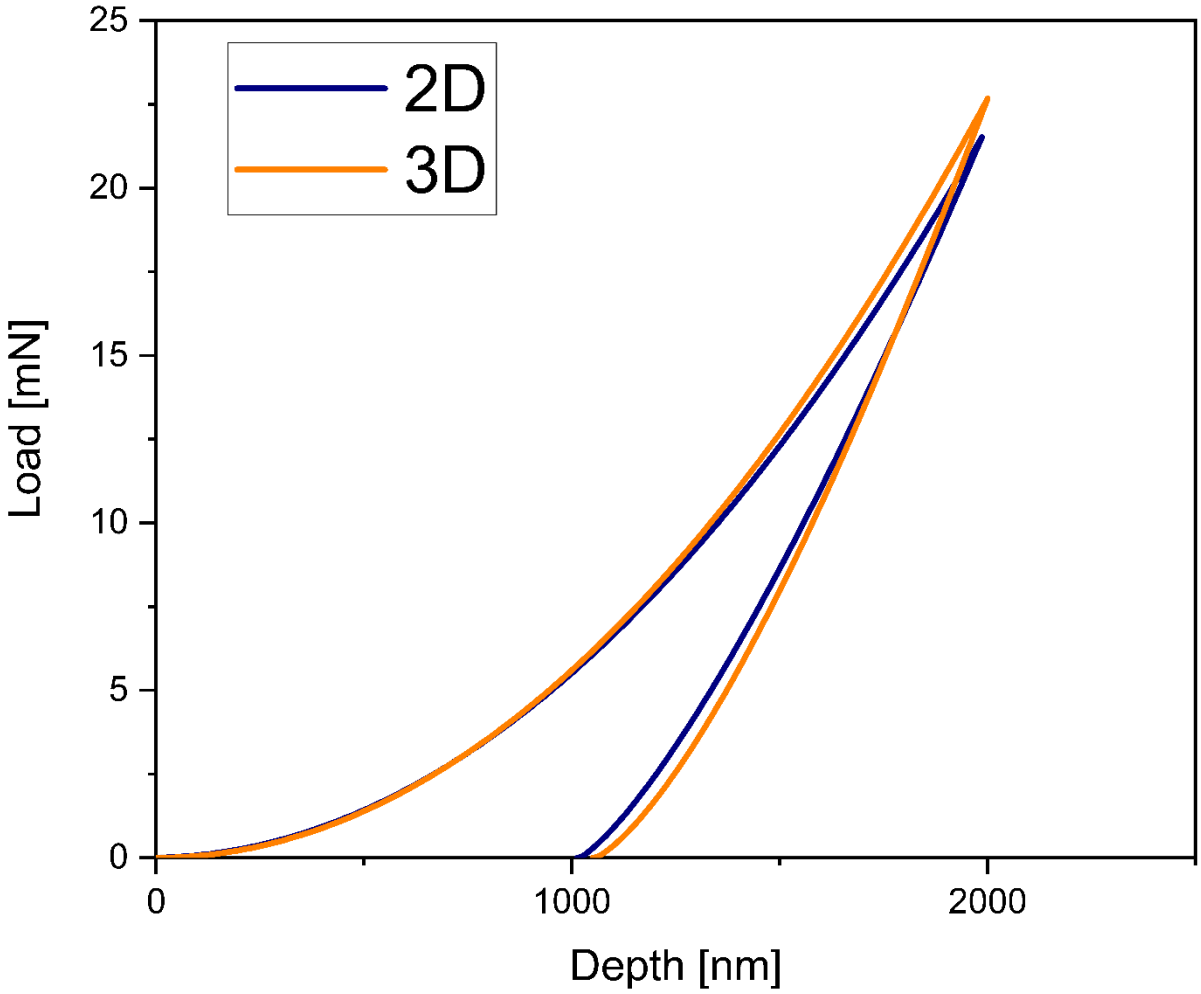

Figure S3. Comparison of the 2D versus 3D finite element models using a Berkovich indenter.

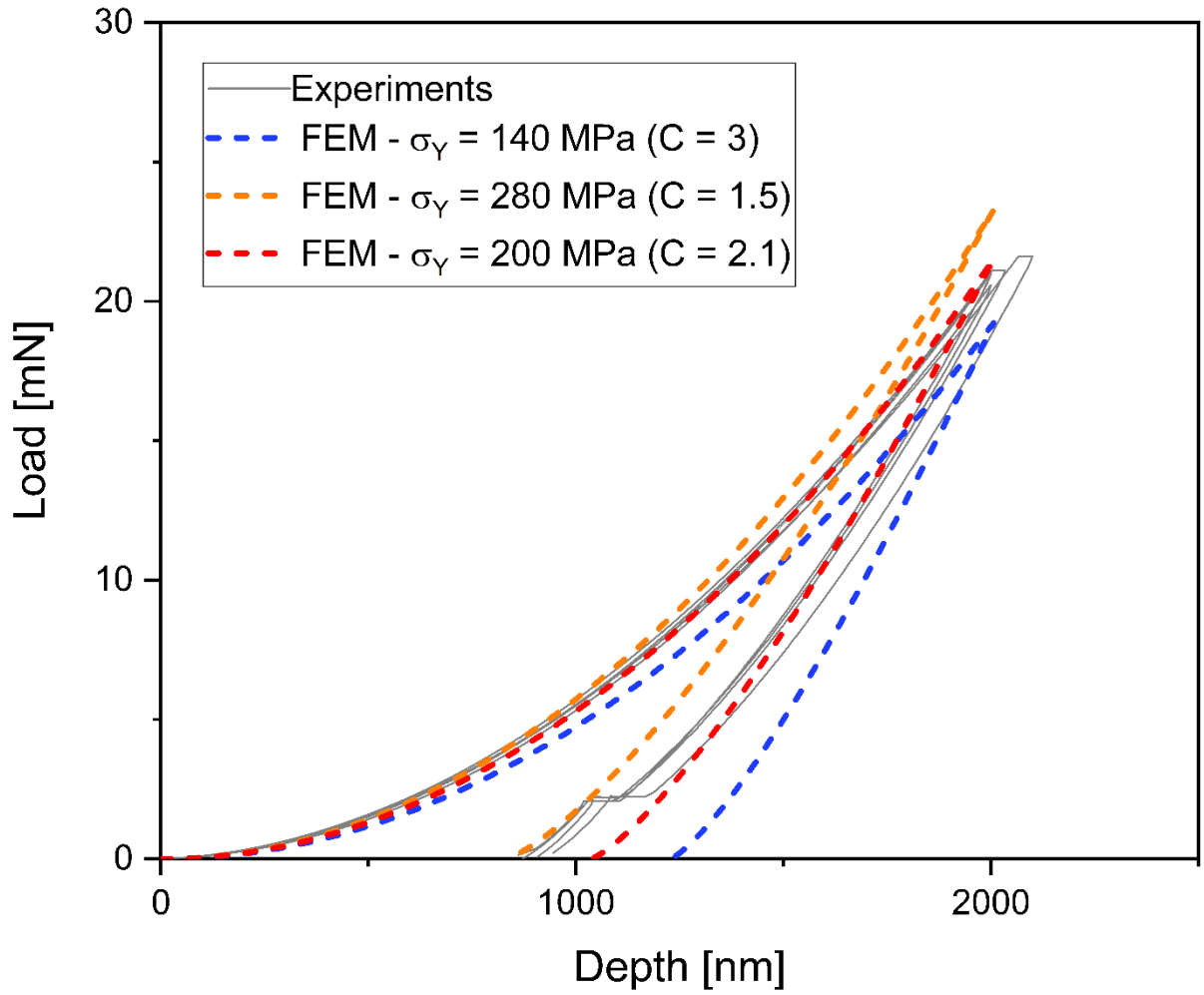

Figure S4. Finite element simulations of Berkovich indentation test of ZIF-8 monolith. The simulation was repeated with different values of the yield strength σ_Y (correspondingly different constraint factors). The best fit with the experiments was achieved with σ_Y = 200 MPa (C= 2.1).

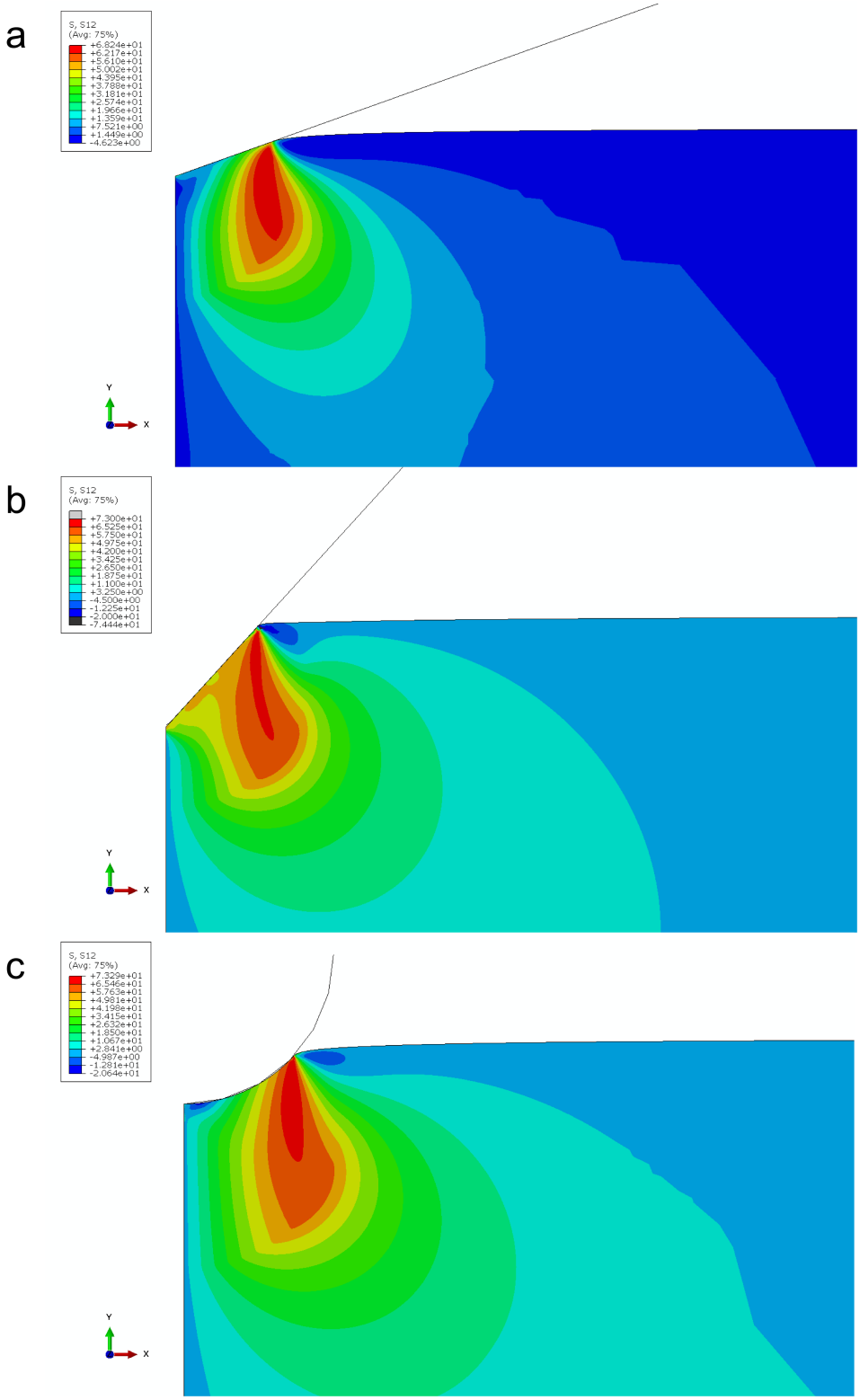

Figure S5. Shear stress contours of the ZIF-71 monolith model at a maximum indentation depth (2000 nm) under the Berkovich (a), cube corner (b), and spherical indenters (c), respectively. The Berkovich and cube corner indenters were modelled as equivalent 2-D cones with semi-apical angles of 70.3˚ and 42.3˚, respectively (see Methods).