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Dynamical Effects in Metal-Organic Frameworks: The Microporous Materials as Shock Absorbers[1] KIETTIPONG BANLUSAN, ALEJANDRO STRACHAN, Purdue University — Metal-organic frameworks (MOFs) are a class of nano-porous crystalline solids consisting of inorganic units coordinated to organic linkers. The unique molecular structures and outstanding properties with ultra-high porosity and tunable chemical functionality by various choices of metal clusters and organic ligands make this class of materials attractive for many applications. The complex and quite unique responses of these materials to mechanical loading including void collapse make them attractive for applications in energy absorption and storage. We will present using large-scale molecular dynamics simulations to investigate shock propagation in zeolitic imidazolate framework ZIF-8 and MOF-5. We find that for shock strengths above a threshold a two-wave structure develops with a leading elastic precursor followed by a second wave of structural collapse to relax the stress. Structural transition of MOFs in response to shock waves corresponds to the transition between two Hugoniot curves, and results in abrupt change in temperature. The pore-collapse wave propagates at slower velocity than the leading wave and weakens it, resulting in shock attenuation. Increasing piston speed results in faster propagation of pore-collapse wave, but the leading elastic wave remains unchanged below the overdriven regime. We discuss how the molecular structure of the MOFs and shock propagation direction affect the response of the materials and their ability to weaken shocks.

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