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Mechanical stability of Metal Organic Framework-5. WEI LIU, JU LI, University of Pennsylvania — Metal organic frameworks (MOFs) are crystalline structures of metal ions bridged by organic linkers. They have been proved to be highly useful in gas storage, separation, purification and catalysis. Mechanical stability is very important for their applications in industry. We studied the stress-strain relations of MOF-5 (the prototypical MOF) under different temperatures via Molecular Dynamics method (MD). It has been found that under normal stress MOF-5 is relatively strong; while under shear stress it is easy to collapse. Furthermore, under both normal and shear stress condition, its stability becomes weaker as temperature increases.

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