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Mechanical modeling of structures exhibiting negative thermal expansion JOSEPH SCHICK, Villanova Univ, ANDREW RAPPE, University of Pennsylvania — Materials that exhibit negative thermal expansion (NTE) over a wide range of temperatures are of great technological importance in creating materials that are structuraly stable despite being exposed to wide variations in operational temperature. One well-known NTE material, ZrW_2O_8, has been the subject numerous investigations and yet the details of the underlying causes of NTE in this material are not resolved. We present results from our theoretical investigation of a mechanical model in which the atoms and their bonds are replaced by point masses and anharmonic potentials. We demonstrate that negative thermal expansion can result solely from the differential expansion of the bonds. Implications for materials design will be discussed.

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