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Inherent Tension in Chemical Bonds¹ JAMES BROCK, QI LIAO, MICHAEL RUBINSTEIN, UNC Chapel Hill, RUBINSTEIN GROUP TEAM — A method is provided for relating average internal tension in bonds between atoms or monomeric units to the external tension applied to them using computer simulations. In dimensions greater than one, there is an average internal tension in bonds on the order of 100 pN even in the absence of an externally applied tension. This non-zero average internal tension is due to asymmetry of thermal fluctuations of bond length and increases with increasing dimensionality. Results from molecular dynamics simulations are in perfect agreement with analytical calculations of tension.

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