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Toward molecular engineering of liquid crystal elasticity: a predictive study of nCB homologues HYTHEM SIDKY, JONATHAN WHITMER, Univ of Notre Dame — The difficulties associated with laboratory measurement of elastic constants present computational methods as an attractive option for understanding the elastic properties of new molecules. Free energy perturbation (FEP) has emerged as a powerful and effective method to obtain liquid crystal elasticities from molecular simulation. However, to date, this method has only been applied to coarse-grained models. Here, we extend this method to the *in silico* measurement of molecular 5CB and its homologues, obtained from simulation using a combination of FEP methods. This represents a milestone in material property prediction and lays the foundation for computationally-guided molecular design of novel mesogenic compounds.

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