Sliding Scales: Tools for predicting and understanding molecular structure from paper and pencil to Beowulf clusters

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Molecular modeling and computational chemistry is sometimes referred to as *in silico* chemistry, evoking notions of molecular ghosts trapped inside silicon computer chips. But not every problem in predicting molecular structure requires a high-performance computer to solve. My research group has been exploring the structures of highly strained and topologically intriguing molecules, including a series of [n] Möbiusenes. What have we learned from using paper and pencil that we could not from a B3YLP/6-31G(d) optimization?