

Abstract Submitted
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The dynamics of a floppy molecule: a case study XIAOJIAN MAO,
Department of Chemistry, West Virginia University — Urea is a simple but interesting molecule. In the solid state it is known to be planar while in gas phase it is non-planar. This difference is attributed to the hydrogen bonding that is present in the solid state. Ab initio quantum calculations suggest that in the gas phase there exist two different non-planar minima: anti- and syn- respectively. In addition to these minima there also exist both rank-one and rank-two saddles separating these minima. In this talk I will discuss topology of the potential energy surface and its implication for the dynamics of the molecule.

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