

Abstract Submitted  
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**Rotational motions in the dynamics of proteins and biological macromolecules** FLORENCE J. LIN, University of Southern California — By changing its shape while conserving angular momentum, a polyatomic molecule can return to its initial shape with a different orientation (as a “falling cat” or a diver can do). Examples where this phenomenon has been observed include the dynamics of protein molecules and the dynamics of a rotary molecular motor. Computational biophysicists have observed the overall rotation of a protein molecule at zero total angular momentum due to the molecule’s flexibility. A counter-rotary motion has been observed in the rotary  $F_o$  motor of ATP synthase. Using geometric mechanics, the net angle of overall rotation is described in terms of coordinates. The net angle of overall rotation is the sum of a dynamic phase and a geometric phase; the latter is also described in terms of a gauge potential. This is an extension of a result for smaller polyatomic systems, where the geometric phase contribution is also described explicitly in terms of moments of inertia and, alternatively, molecular rotational constants. Potential applications of this result include computational molecular dynamics studies.

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