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# The Extension of Monomeric Computational Results to Polymeric Measurable Properties: An Introductory Computational Chemistry Experiment

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**Abstract :** Advances in software technology enable computational chemistry to be commonly applied in various research fields, especially in pedagogy. Thus, in order to expand and improve experimental instructions of computational chemistry for undergraduates, we designed an introductory experiment—research on acrylamide molecular structure and physicochemical properties. Initially, students construct molecular models of acrylamide and polyacrylamide in Gaussian and Materials Studio software respectively. Then, the infrared spectral data, atomic charge and molecular orbitals of acrylamide as well as solvation effect of polyacrylamide are calculated to predict their physicochemical performance. At last, rheological experiments are used to validate these predictions. Through the combination of molecular simulation (performed on Gaussian, Materials Studio) with experimental verification (rheology experiment), learners have deeply comprehended the chemical nature of acrylamide and polyacrylamide, achieving good learning outcomes.

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