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Undergraduate research for molecular bond measurements[1] DAYTON BROWN, JOSEPH YANG, VOLA M ANDRIANARIJAONA, Department of Physics, Pacific Union College Angwin CA 94508 — When studying molecules it is useful to calculate the energetics, atomic spatial positions relative in three dimensions, and the vibrational frequency of each bond. Due to the huge number of particles, the sheer number of interconnected bonds, and the complexity in large biological molecules, simplifications and approximations are required for the calculations and estimations of useful data. To calculate ionization energy for a particular geometry of a molecule, we use the free version of ORCA [1], a program based on Density Functional Theory (DFT), and use the results as tools to quantify physical and chemical properties of various biological compounds including basic compounds such as water. The applications of these research tools can be easily extended to the study of large biomolecules such as amino acids. Amino acid interactions cause proteins to fold in specific manners. Basic properties such as ionization energies shed lights on these interactions, thus they are useful for studying diseases where proteins misfold and produce cellular problems. Few examples, including the different steps are shown in this poster.
[1] F Neese, "The ORCA program system". Wiley Interdisciplinary Reviews: Computational Molecular Science 2 (1), 73-78

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Dayton Brown
Department of Physics, Pacific Union College Angwin CA 94508

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