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Developing Potential Energy Curves of Acidic and Basic Amino Acids Using Quantum Computational Techniques C.P. DE GUZMAN, M. ANDRIANARIJAONA, Y. YOSHIDA, K. KIM, V.M. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA 94508 — Proteins are made out of long chains of amino acids and are an integral part of many tasks of a cell. Because the function of a protein is caused by its structure, even minute changes in the molecular geometry of the protein can have large effects on how the protein can be used. This study investigated how manipulations in the structure of acidic and basic amino acids affected their potential energy. Acidic and basic amino acids were chosen because prior studies have suggested that the ionizable side chains of these amino acids can be very influential on a molecule's prefered conformation. Each atom in the molecule was pulled along x, y, and z axis to see how different types of changes affect the potential energy of the whole structure. The results of our calculations, which were done using ORCA, emphasize the vibronic couplings. The aggregated data was used to create a data set of potential energy curves to better understand the quantum dynamic properties of acidic and basic amino acids (preliminary data was presented in http://meetings.aps.org/Meeting/MAR16/Session/M1.273 and-http://meetings.aps.org/Meeting/FWS16/Session/F2.6).

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