Abstract Submitted
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Calculating the Ionization Energies of Acidic and Basic Amino Acids Through the Analysis of Potential Energy Surfaces C. P. DE GUZMAN , M. ANDRIANARIJAONA, Y. YOSHIDA, V. M. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA 94508 — Strain on the molecular geometry of amino acids can have varying effects on the amino acid's structure, function, and overall binding capabilities. A better understand of how strain affect the potential energy can also lead to more insight to a molecule's vertical ionization energy. For this study, acidic and basic amino acids were chosen because of their ionizable side chains are very influential on the molecule's preferred conformation (J Phys Chem A. 2011 April 7; 115(13): 2900–2912). Each atom within the amino acid was considered as potential departing sites to better understand the dynamic coupling between the vibrational modes. ORCA was used to calculate single point energies after manipulating the location of each atom along the x, y, and z coordinates. The collected data was then used to create potential energy surfaces to better understand the quantum dynamic properties of the amino acids (preliminary data was presented in http://meetings.aps.org/Meeting/MAR16/Session/M1.273).

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