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Quantum Computational Calculations of the Ionization Energies of Acidic and Basic Amino Acids: Aspartate, Glutamate, Arginine, Lysine, and Histidine.[1] C. P. DE GUZMAN, M. ANDRIANARIJAONA, Y. S. LEE, V. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA, 94508 — An extensive knowledge of the ionization energies of amino acids can provide vital information on protein sequencing, structure, and function. Acidic and basic amino acids are unique because they have three ionizable groups: the C-terminus, the N-terminus, and the side chain. The effects of multiple ionizable groups can be seen in how Aspartate's ionizable side chain heavily influences its preferred conformation (*J Phys Chem A.* 2011 April 7; 115(13): 2900–2912). Theoretical and experimental data on the ionization energies of many of these molecules is sparse. Considering each atom of the amino acid as a potential departing site for the electron gives insight on how the three ionizable groups affect the ionization process of the molecule and the dynamic coupling between the vibrational modes. In the following study, we optimized the structure of each acidic and basic amino acid then exported the three dimensional coordinates of the amino acids. We used ORCA to calculate single point energies for a region near the optimized coordinates and systematically went through the x, y, and z coordinates of each atom in the neutral and ionized forms of the amino acid. With the calculations, we were able to graph energy potential curves to better understand the quantum dynamic properties of the amino acids.

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