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Binding Affinities of Selected Aliphatic A-Amino Acids with Graphene: A Computational Study

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Density functional theory (DFT) calculations were performed to understand the binding of eight aliphatic amino acids (glycine, alanine, valine, leucine, cysteine, methionine, aspartic acid and glutamic acid) individually with two finite size graphene sheets. After performing conformational analysis for these eight amino acids using Merck Molecular Force Field (MMFF) implemented in Spartan '18 software package, geometries of all the conformers were refined first at the HF/6-31G (d) level and then at the M06-2X/6-31G (d) level. The most stable conformer obtained at the M06-2X/6-31G (d) level was used to build complexes with graphene by considering different possible binding modes. All the complexes were fully optimized using M06-2X/6-31G (d) level. Binding energies with and without basis set super position error (BSSE) corrections were calculated and analyzed. Our study reveals that multiple C-H…pi and N-H…pi interactions contribute for stabilization of the complexes. The data obtained from our computational study may be helpful for force field development and for future experiments on non-covalent interactions of amino acids with graphene. Our findings would provide insights for experiment a lists exploring graphene nanomaterials for potential applications in drug delivery, biomedical implants (or biocompatible materials), biomedical imaging, protein sequencing and biosensor devices. Our goal is to understand the relationship between the binding affinities of various complexes and structural features including the orientation of amino acid adsorbed on varying sizes of graphene surface.

Biography:

Jovian is currently a Ph.D. student in chemistry at Clark Atlanta University (CAU). He earned his B.S. in chemistry from Savannah State University. While attending CAU, he achieved several prestigious awards such as Extreme Science and Engineering Discovery Environment (XSEDE) Scholar in 2016, XSEDE travel award for PEARC17 conference and Mickey Leland Energy Fellowship (MLEF)-U.S., Department of Energy (DOE) in summer of 2018. Some of his research interests are computational design of materials, nanomaterials-based alternative energy, solar energy harvesting and utilization of electrochemistry for conversion of environmental gases. After graduation, he plans to take a postdoc position preferably at a national lab.