UNIVERSITI TEKNOLOGI MARA

SIMULATION STUDY ON STRUCTURAL AND ELECTRONIC PROPERTIES OF UREA AND HYDROXYAPATITE AS SLOW-RELEASE FERTILIZER BY USING DENSITY FUNCTIONAL THEORY (DFT)

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ABSTRACT

Nitrogen and phosphorus are the macronutrients crucial for the crops' growth. Due to the environmental factors, these nutrients are easily washed away before reaching the crops. Slow-release fertilizer was created to address this problem by gradually releasing nutrients to the plants. This thesis is on the theoretical work, using density functional theory (DFT), to study the intricacy of the interaction between urea and hydroxyapatite in terms of relative stability, structural and electronic properties. Gaussian 09 suite program and Multiwfn software were utilized in analyses these properties at level B3LYP/6-31G(d,p). The HA crystal structure was divided into three clusters: HA1 (no hydrogen atoms), HA2 (hydrogen atoms), and HA3 (a mixture of HA1 and HA2). ESP displayed the minimum points near the abundant hydrogen atoms while the maximum points were located near the oxygen and calcium atoms. The urea molecules were moved from the yellow or red region to the blue region on HA surfaces, and their position was changed from horizontal to vertical. For comparing the calculated interaction energy, B-HA1 and C-HA3 were the most stable combinations across all the basis sets. For HA2, B-HA2 was more stable at 6-31G(d,p) and 6-311++G (2df,2pd), while for DEF2-TZVP, C-HA2 was more stable. Topology analysis displayed new bonding formed between nitrogen, hydrogen and oxygen in urea with calcium, oxygen and hydrogen in HA for all combinations. Strong attraction, vdW interaction and low electron density of colored slab are visible between new bonds on NCI isosurfaces. In ELF color map, the stable combinations have ELF values within 0.04 to 0.26, which represent perfect delocalization. Based on variations in wavenumbers, new interactions of bonding had formed between urea and HA. HA2 is the most stable structure with large energies gap of 1.1439 eV between HOMO and LUMO. All the HOMO and LUMO lobes were found near calcium atoms, hydrogen atoms and oxygen atoms in all HA clusters and stable combinations.

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