Engineering Solid Mechanics

Comparative study of graphene-polypyrrole and borophene-polypyrrole composites: Molecular dynamics modeling approach

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Abstract

In the search for the solution to energy storage problems, this study investigates the interfacial energy interaction and temperature stability of the composites made of polypyrrole-graphene-borophene (PPy-Gr-Bon) by using molecular dynamics simulations. From the calculated thermodynamics and interfacial energies of the system, comparisons between the ternary and the binary-binary systems were made. The materials in the entity show a good degree of temperature stability to a dynamic process at 300, 350, 400, and 450 K. Moreso, at 300 K, the interaction energy of PPy-Gr, PPy-Bon, and PPy-Gr-Bon are: -5.621e3 kcal/mol, -26.094e3 kcal/mol, and -28.206e3 kcal/mol respectively. The temperature stability of the systems is in the order of: PPy-Gr-Bon > PPy-Bon > PPy-Gr. The effect of temperature on the interaction energy of the systems was also investigated. The ternary system showed higher stability as the temperature increased. In addition, the radial distribution function computed for the three systems revealed that there is a strong, but non-chemical bonding interaction between PPy-Gr-Bon, Bon-PPy, and Gr-PPy. By considering the excellent mechanical properties of PPy-Gr-Bon and the already established high electrical conductivity and chemical stability of Gr, Bon and PPy, their composite is therefore suggested to be considered for the manufacturing of electrochemical electrodes.