MOLECULAR SIMULATIONS OF NANO-STRUCTURED CARBON

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ABSTRACT

Nano-structured carbon materials exhibit many interesting properties and have been applied in diverse areas. However, it is challenging to extract atomic-level structural information (short- and medium-range ordering for amorphous nano-structured carbon or defects structure for crystalline nano-structured carbon) via the available experimental techniques. The lack of structural understanding of nano-structured carbon prevents us to develop structure-property understanding of these materials. In this dissertation, we endeavor to tackle this problem using the virtual synthesis technique to obtain realistic atomic models for nano-structured carbon. In particular, we obtained nanoporous carbon from simulated pyrolysis (NPC-SP), nanoporous carbide-derived-carbon from carbon reduction (NPC-CDC) and graphene from chemical vapor deposition (CVD) growth on copper. We demonstrate the usefulness of the model nano-structured carbon from virtual synthesis by investigating the transport property of NPC and various applications of graphene at the solid-liquid interfaces.