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Molecular Dynamics Study on Core-Shell Structure Stability of Aluminum Encapsulated by Nano-carbon Materials

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Abstract

A ReaxFF reactive forcefield for aluminum-carbon composite system has been developed to investigate structural stability and thermal decomposition mechanism of nano-carbon materials coating aluminum particles. Research results indicated the Al@C particles were structurally stable in a broad temperature range from room temperature up to 2735K. In particular, the broken carbon cage self-healed to reconstruct a more stable Al@C core-shell structure after Al atoms sequentially departing from carbon cage during thermal decomposition, proffering an effective protection for aluminum surface-activeness.

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