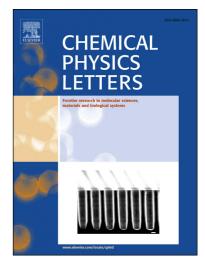
Accepted Manuscript

Research paper

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PII:	S0009-2614(16)30962-9
DOI:	http://dx.doi.org/10.1016/j.cplett.2016.12.013
Reference:	CPLETT 34380
To appear in:	Chemical Physics Letters
Received Date:	12 October 2016
Revised Date:	14 November 2016
Accepted Date:	7 December 2016



Please cite this article as: Q. Yi, J. Xu, Y. Liu, D. Zhai, K. Zhou, D. Pan, Molecular Dynamics Study on Core-Shell Structure Stability of Aluminum Encapsulated by Nano-carbon Materials, *Chemical Physics Letters* (2016), doi: http://dx.doi.org/10.1016/j.cplett.2016.12.013

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ACCEPTED MANUSCRIPT

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. Download English Version:

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