

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Why the Mechanical Properties of Cross-linked Polydimethylsiloxane Surface Enhance? – A First Principles Study** ZHIFAN WANG, MENGTING JIN, YANNING ZHANG, Chengdu Green Energy and Green Manufacturing Technology RD Center , BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER COLLABORATION — Polydimethylsiloxane (PDMS) has been widely used in various areas due to its high flexibility, controllable mechanical properties, brilliant biocompatibility and low cost. Now more work on PDMS focus on tuning its surface physical and chemical properties. Our experimental group has shown that the top surface stiffness of PDMS is significantly enhanced after a surface treatment of hyperthermal hydrogen induced cross-linking (HHIC), without losing its inherent hydrophobicity. To understand why this, we investigated how the HHIC treatment changes the structure of PDMS molecules and chains, by using density functional theory (DFT) calculations with the nonlocal van der Waals interaction. The elastic and hydrophobic properties of PDMS, before and after the surface treatment, will be discussed then, providing deep understandings on the experimental observations. Our theoretical studies could give insights in the new development of HHIC tuning technology.

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Date submitted: 04 Nov 2015

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