



Plaform: Nano/Energy



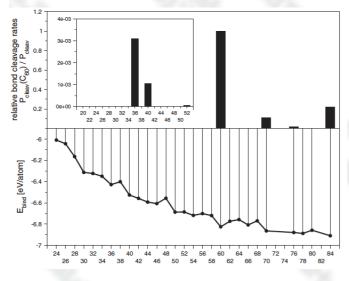
Theoretical Chemistry Colloquium

July 3, 2013 (Wed), 16:00-17:00

RCMS, 2nd floor, Chemistry Gallery

Kinetic stability vs thermodynamics of nanostructures - investigation of relative stability of fullerenes and SWCNTs

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Abstract: A model to evaluate kinetic stability of caged carbon nanoclusters was developed based on assumption of independent and random nature of thermal vibrations of atoms. Probabilities of breaking of carbon-carbon bonds in fullerenes and SWCNT were determined and clear inverse correlations of maximal probabilities with experimental isomer relative yields were found. It was shown that the carbon cage abundance is governed by kinetic rather than thermodynamic stability.



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