Nanocomposites and nanomaterials

Ab-initio simulation of the atomic structure and mechanical properties of carbyne

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Recently, linear monatomic chains or carbyne were intensively investigated due to their unique physical properties [1, 2] and promising applications [3, 4], but the possibility of realization their properties is limited by their strength and elasticity.

This paper presents the results of *ab-initio* modeling of structure and mechanical properties of a monatomic linear chains containing 2÷20 atoms. For chain with number of atoms $N \geq 10$, the existence of stable cumulene-structure in the inner part of the chain was ascertained. Stabilization of cumulene-structure can be considered as a result of strong edge effect in finite chains. This is the fundamental difference between the finite and infinite chain, for which polyyne-structure is stable. Stress-strain curves are obtained for different atomic chains. It enabled to determine the value of strength, fragility and elastic modulus. For chains with $N \geq 4$, the relation between strength and binding energy in chains is established. The strong scale effect and the effect of parity are shown for strength and binding energy. Chains with an odd number of atoms are stronger and less brittle than the "even" chains. Chains with 5 atoms have maximum strength that is equal to 13nN. All these effects disappear when the number of atoms in the chain is greater than 10. ".

1. *L. Ravagnan et. al. // Phys. Rev. Lett. 102, 245502.*
2. *E. Cinquanta, L. Ravagnan, I. E. Castelli, F. Cataldo, N. Manini, G. Onida, and P. Milani // J. Chem. Phys. 135, 194501.*
3. E. E. Durgun, R. T. Senger, H. Mehrez, S. Dag, and S. Ciraci // Europhys. Lett. 73, 642 (2006).
4. Y. Wang, X.-J. Ning, Z.-Z. Lin, P. Li, and J. Zhuang // Phys. Rev. B 76, 165423 (2007).