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PS2-26: Study Elastic Properties of the Carbyne Method of Molecular Dynamics

Tuesday, 7 October 2014 17:00 (1h 30m)

We study the mechanical properties of the carbene. Model is an array of long chains of 13 nm, located in the cell with periodic boundaries on the sides. At a temperature of 300K, the model is the longitudinal tension. Results on the change of the interatomic bonds, calculated Young's modulus ≈ 0.15 TPa whose order is consistent with the recently published work [1].

References

1. A.K. Nair, S.W. Cranford and M.J. Buehler, EPL, 95 (2011) 16002.

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