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First-principles calculations of channeling of low-energy ions in SWCNTs and the effect of many-particle interactions

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Previously, calculations showed that the channeling of low-energy ions in SWCNTs leads to the emergence of many-particle interactions, which leads to the establishment of a special regime of particle motion in the SWCNT channel, similar to gliding [1]. In this work, using TD-DFT [2] and ab initio molecular dynamics [3] methods, a similar mechanism was considered, taking into account many-particle interactions from first principles.

The model is based on the PBE functionality; the STO-3G and 6-31G basis sets were used.
The research is carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University [4].

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