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Predicting molecular excitations induced by a high-velocity massive charged particle

The objective of the conducted research was to develop a quantum chemical method that enables modeling of interactions between high-velocity, massive, charged particles and an arbitrarily chosen molecule. The proposed method finds broad application across various fields of science. In the context of radiotherapy, a tool capable of accurately describing excitations induced by protons is highly desired to calculate the rate of energy transfer from the high-velocity particle to tissues [1]. Simultaneously, the ability to predict transition probabilities between molecular electronic states, induced by massive, charged particles, can significantly contribute to the development of high-energy physics, particularly in the search for particles that could potentially constitute dark matter [2]. This study focused on the second of the mentioned applications. Two alternative approaches to modeling the interaction between a particle and a molecule were presented, both based on the time-dependent perturbation theory formalism. The massive, charged particle was treated as a classical point particle generating a standard electric potential. The main focus was placed on molecular excitations, neglecting processes such as ionization or electron capture. Excitation probabilities were calculated for water molecules, LAB (linear alkylbenzene) molecules, and argon atoms, induced by a hypothetical dark matter particle (gravitino). In calculations, two possible velocities were investigated, corresponding to a gravitino bound to the Solar System or the Milky Way Galaxy. Excitation cross sections and characteristic times between excitations were presented for both of them. The results enable the prediction of the gravitino's signature in the analyzed detectors. Moreover, it was demonstrated that detectors containing LAB are the most suitable for conducting this type of experiment [3].

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