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(54) Title: METHOD FOR LARGE TIMESTEPS IN MOLECULAR MODELING

(57) Abstract: For the computer modeling of molecules, a model with reduced coordinates is used with sufficiently stable implicit integration methods integrating the model's equations of motion. The timesteps in the integration method can vary in a range over 100 to greatly increase the computer's efficiency and to hasten the computational results. Both static analysis and molecular dynamics simulations are some ready applications.

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