Molecular dynamic studies on the evolution of Al$_8$Cu$_4$Fe$_1$, Al$_{27}$Cu$_{10}$Fe$_5$ and Al$_{34}$Cu$_{14}$Fe$_7$ Icosahedral quasicrystal using DFT

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Computer simulation methods, such as monte carlo or molecular dynamics, are very powerful computational techniques that provide detailed and essentially exact information on classical many-body problems. Evolution of Icosahedral quasicrystal Al$_8$Cu$_4$Fe$_1$, Al$_{27}$Cu$_{10}$Fe$_5$ and Al$_{34}$Cu$_{14}$Fe$_7$ clusters were presented. It was observed the fluctuations of total energies and conserved Hamiltonian was due to potential energy and kinetic energy respectively. Also stability behavior due to the instantaneous temperature makes the thermostat efficient. However, Ir-spectrum extracted from the trajectories of the fourier transform of the dipole-dipole auto-correlations are presented and are in agreement with Mansur and Babaji, 2016 and Rudenko and Mazurenko 2007.

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