

# Electronic structure of nanosystems by quantum Monte Carlo methods

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The talk will be focused on recent developments in quantum Monte Carlo methods for electronic structure calculations and their applications to nanostructure systems. This will include methods for evaluation of interatomic forces in correlated wave function framework and QMC calculations of excited states and optical response in clusters. The applications will be focused on competition between aromaticity and second-order Jahn-Teller effects in Huckel carbon rings, formation energies of protonated hydrogen clusters, optical response of both doped and undoped silicon nanocrystals and studies of the smallest heteroatom fullerenes. The references can be found at the webpage [1].

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[1] <http://altair.physics.ncsu.edu/lubos/main.html>.