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Interplay between rotational dynamics, quantum solvation and superfluid response in doped helium clusters

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We show how state-of-the-art Quantum Monte Carlo methods assist in revealing the interplay between rotational dynamics, quantum solvation and superfluid response in doped helium clusters. While strong correlations exist between the size variation of the rotational constant and changes in structure, exchange effects are crucial to explain a non-monotonic evolution of the rotational constant of the complexes. We demonstrate that exchanges facilitate the decoupling between a dopant molecule and helium for cluster sizes where the effective anisotropy of the helium-dopant interaction is reduced due to structural changes. In addition, for the class of molecular dopants with a T-shaped He-molecule dimer configuration, the variations in the rotational constant can be unambiguously related to the non-trivial evolution of the helium superfluid response. This allows one to use a molecular dopant as an experimental probe of superfluidity at the microscopic level. We show that experimental superfluid response builds up in stages correlated with the filling of the solvation layers around the dopant molecule.