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# The cationic lithium dimer solvated in He clusters: Molecular Dynamics Simulations.

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The structures and energetics of Li+2-doped He clusters have been determined by means of evolutionary programming optimizations and classical molecular dynamics simulations [1]. The underlying interactions in the HeN Li+2 complexes are described by sum-of-potentials ab initio-based models [2]. The classical picture of the He atoms surrounding the cationic dimer shows a selective growth of the clusters. Figure below shows a contour plot of the probability distribution in the (z, ρ)-plane (right panel) and classical thermal conformer (left panel) for the N=30 cluster at T=2 K. The z axis is along the cationic dimer. Using the Feynman-Hibbs second order approach [3], quantum results are also presented and discussed.

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