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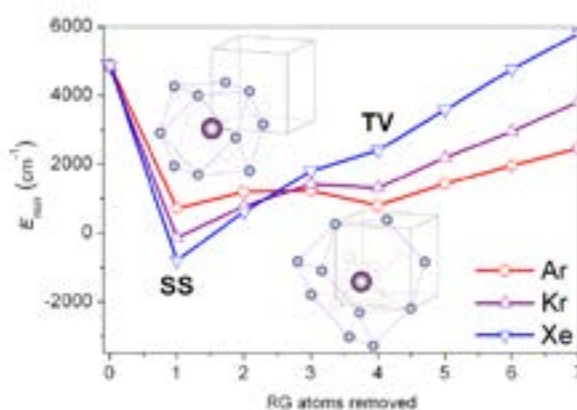
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## Atoms and dimers in rare gas crystals: Modeling of the stable trapping sites

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Matrix isolation spectroscopy of atomic and small molecular species regularly and reproducibly reveals the existence of distinct trapping sites, sometimes undergoing reversible and irreversible interconversion processes upon heating or irradiation. While the modeling of trapping site structures as the minima on the potential energy surface is a mature task, assessment of thermodynamic stability implies the consideration of ensembles of structures thus requiring special efforts. Recently, we have proposed the model compatible with the thermodynamic phase stability analysis. Assuming a crystalline matrix, the model, first, compromises its local distortions by embedded host and long-range crystal order. Second, the correction to atomization energy allows one to consider the structures of distinct nature – insertions, substitutions and vacancy formations – at the same energy scale. Resulting dependence of the energy on the number of host atoms removed from the system makes it possible to use the convex hull concept to identify thermodynamically stable site structures. The figure exemplifies such dependences for Mn atom trapped in Ar, Kr and Xe, as calculated using the *ab initio*-based pairwise interaction potentials. It illustrates stabilization of the single substitution (SS) site and destabilization of the tetra vacancy (TV) one with the size of host atom, in agreement with recent spectroscopic data. Application of the model to Mn<sub>2</sub> molecule has revealed that the matrix accommodates this weakly-bound dimer per atom, merging stable atomic SS and TV structures within the single unit cell. These sites are discernible by vibrational frequencies and spin-spin coupling parameters. Other examples of trapped species are also considered. Identification of the thermodynamically stable trapping site structures provides the grounds for interpreting slow heat- and light-induced processes in cryogenic matrices and facilitates accurate spectroscopic and dynamical simulations of the matrix isolated species.



### Biography

Alexei Buchachenko is the Professor at Skolkovo Institute of Science and Technology in Moscow, Russia and also holds Part-time Professor Position in Department of Chemistry at Moscow State University. His research interests are connected with the theoretical studies of structure, spectroscopy and dynamics of small molecules, recently with applications atomic, ionic and molecular systems at low temperatures.

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