

Atoms and Molecules in a Confined Environment

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It is known that quantization arises from imposing boundary conditions, the classic example being a particle in a box. The talk will illustrate how properties of atoms and molecules change because of confinement, using endohedral fullerenes as examples. For example, the stretching frequencies of molecules like water and ammonia confined to a fullerene (C_{60}) cage exhibit a blue shift. Hydrogen bond between water molecules breaks inside the cage. Although small molecules like B_2 and O_2 retain their paramagnetic property, Ge_2 exhibits a spin cross over as it rotates inside the cage. The noncovalent interaction between rare gases undergoes a quantitative change due to confinement inside a carbon nanotube. The molar heat capacity of fullerene (C_{60}) changes due to encapsulation of rare gas atoms by $0-3R$ over a temperature range.

References

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