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## CHEMICAL PHYSICS OF FREE MOLECULES - Springer

chemical bonding in free molecules. (For the reader who becomes deeply interested in the electron density description, advanced accounts can be found in *The Theory of the Inhomogeneous Electron Gas*, S. Lundqvist and N. H. March, eds.,

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Chemical physics of free molecules by Norman H. March, 1993, Plenum Press edition, in English

### Chemical physics - Wikipedia

Chemical physics is a subdiscipline of chemistry and physics that investigates physicochemical phenomena using techniques from atomic and molecular physics and condensed matter physics; it is the branch of physics that studies chemical processes from the point of view of physics.

### Monte-Carlo simulation and mean-field theory ...

In the above equation  $U_{0A}$  and  $U_{0B}$  are free energies of adsorption for methane and ethane molecules, respectively, interacting with the lattice. These two phenomenological parameters can include changes in ro-vibrational free energies on adsorption of an isolated molecule onto the zeolite lattice from the gas phase.

### The chemical potential of water: molecular dynamics ...

The method of thermodynamic integration has been used to calculate the free energy difference between the (model) water and an ideal gas of molecules at the same temperature and volume. For this particular thermodynamic property, Ewald sums and truncated potentials yield the same results.