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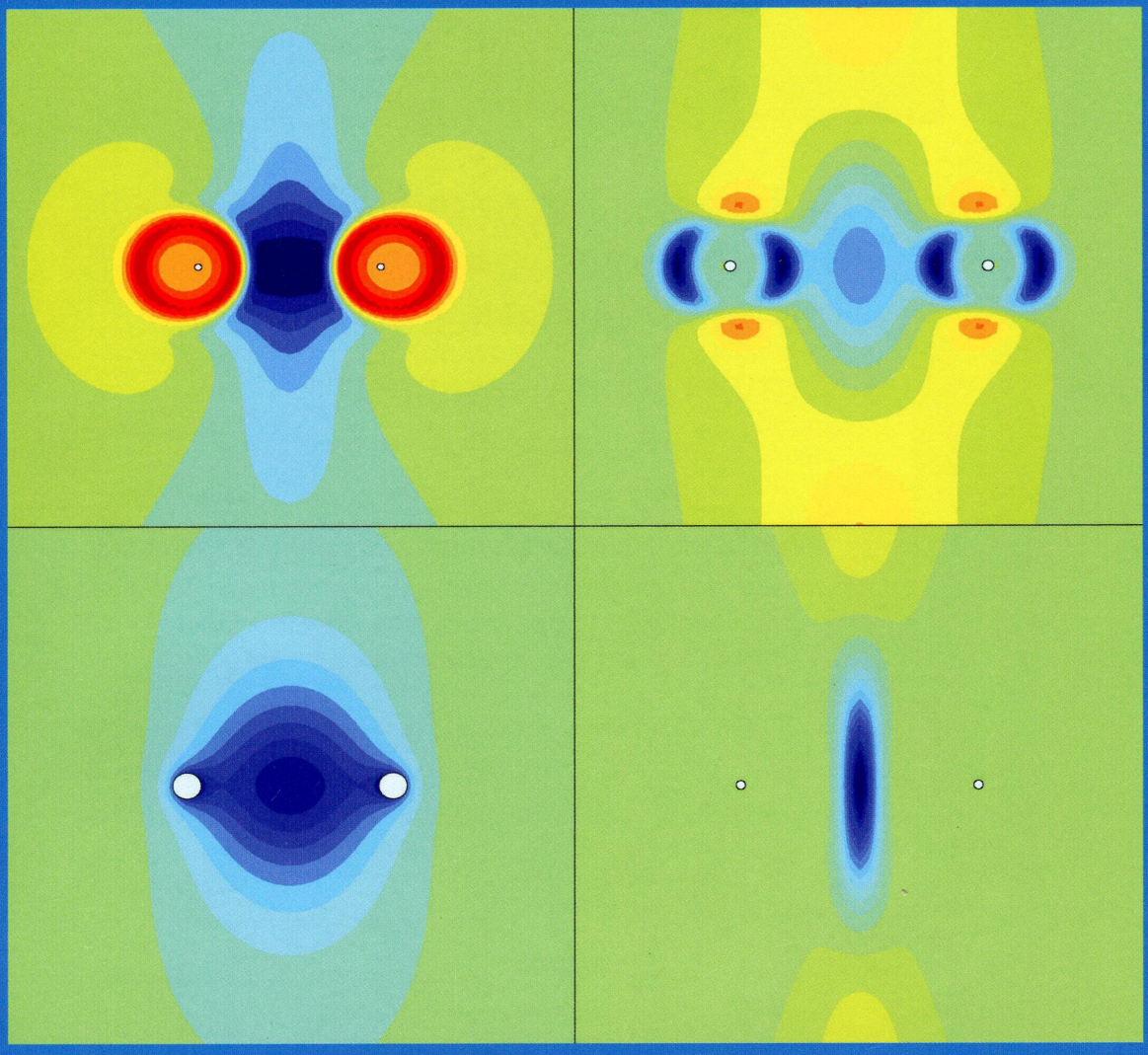

Partition Potentials for the First Four Homonuclear Diatomics. Clockwise from Top Left: Li_2, Be_2, He_2, H_2
(see page 5A)

ISOLATED MOLECULES, CLUSTERS, RADICALS, AND IONS; ENVIRONMENTAL CHEMISTRY, GEOCHEMISTRY, AND ASTROCHEMISTRY; THEORY

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ON THE COVER: The cover displays plots of partition potentials for the first four homonuclear diatomic molecules. Clockwise from top left: Li_2, Be_2, He_2, H_2. The partition potential is a molecular fingerprint provided by partition density-functional theory (PDFT). It is the global one-body external potential that, when added to each of the nuclear potentials of the isolated fragments, deforms their electronic densities so that their sum is exactly the molecular density obtained from a Kohn−Sham (KS) calculation (the local density approximation was used for the potentials shown here). See page 7623.

Feature Article

Articles

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Molecular Structure, Quantum Chemistry, and General Theory

Additions and Corrections

Ⓢ Supporting Information available via online article