**The Nearly Degenerate Triplet
Electronic Ground State
Isomers of Lithium Nitroxide**

Justin M. Turney and Henry F. Schaefer III
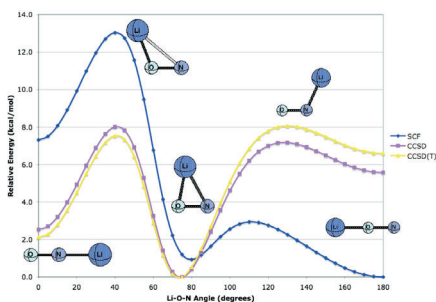
**A Fundamental Relation of Molecular
Informatics on the Information-Carrying
Properties of Density Functions**

Paul G. Mezey

Holographic
Electron $\Rightarrow$ Molecular
Density   Informatics

**A Note About the Ground State
of the Hydrogen Molecule**

Alexander V. Turbiner and
Nicolais L. Guevara

$$\psi^{(\text{trial})} = A_1\psi_1 + A_2\psi_2 + A_3\psi_3$$

$$\psi_1 = (1 + P_{12})(1 + P_{AB})\, e^{-\alpha_1 r_{1A} - \alpha_2 r_{1B} - \alpha_3 r_{2A} - \alpha_4 r_{2B} + \gamma_1 r_{12}}$$
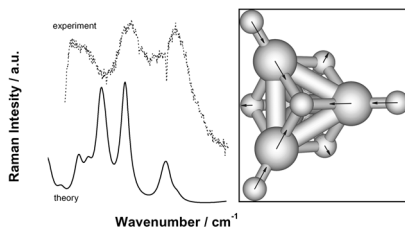
$$\psi_2 = (1 + P_{12})\, e^{-\alpha_5 (r_{1A} + r_{2B}) - \alpha_6 (r_{1B} + r_{2A}) + \gamma_2 r_{12}}$$

$$\psi_3 = (1 + P_{12})\, e^{-\alpha_7 (r_{1A} + r_{1B}) - \alpha_8 (r_{2A} + r_{2B}) + \gamma_3 r_{12}}\ .$$

**Raman Spectroscopy of Nanocrystalline
Li-Ti-O Spinels and Comparative DFT
Calculations on Ti_yO_z and $Li_xTi_yO_z$
Clusters**

Jakub Jirkovský, Kateřina Macounová,
Hartmut Dietz, Waldfried Plieth, Petr Krtil and
Stanislav Záliš

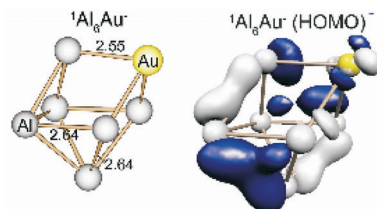### On the Magic Character of Al_6Au^-

Michele L. Kimble, Albert W. Castleman, Jr.,
Jose U. Reveles and Shiv N. Khanna

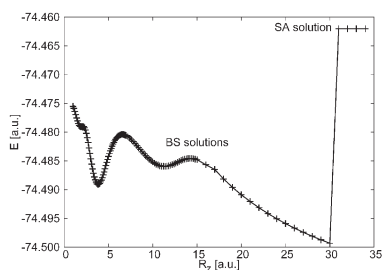### Hartree–Fock Stability and Broken Symmetry Solutions of O^{2-} and S^{2-} Anions in External Confinement

Filip Holka, Pavel Neogrády,
Miroslav Urban and Josef Paldus

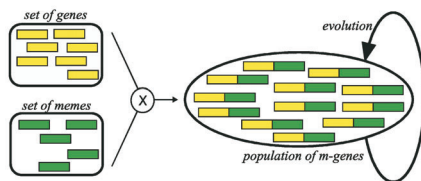### Artificial Chemistry and Replicator Theory of Coevolution of Genes and Memes

Vladimír Kvasnička and Jiří Pospíchal

The Quantum Mechanics of Cohesion

Roy McWeeny

$$H_{spin} = E_0 + E_1(\mathbf{S}^A \cdot \mathbf{S}^B) + E_2(\mathbf{S}^A \cdot \mathbf{S}^B)^2 + \dots$$

The Absolute Entropies of Alkali Metal Borides. Simple Patterns and High-Level Calculations

Ivan Černušák, Martina Čukovičová, Alexandra A. Asiama, Susan K. Gregurick, Paul A. Hoover, Sarah C. Tsay and Joel F. Liebman

$$S^\star(XY) = 1/2[S^\star(X_2) + S^\star(Y_2)]$$

Quantum Effects on the Caloric Curves of Lithium Clusters

Fernand Spiegelman and Florent Calvo

(a) Li_{20} - TB