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Don McQuarrie's research interests were in theoretical chemistry, specifically in statistical thermodynamics of electrolyte systems and transport through membranes, stochastic differential equations, and nonlinear dynamical systems.

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Contrasting LCAO with other Quantum Chemistry Methods. As we have already seen, the LCAO approach is very approximate, yielding only qualitative results. It should be noted that the Hartree-Fock method discussed earlier for atoms can also be used for molecules. For example, the molecule $(\text{He}_2)^{+}$ has three electrons, and the Li atom also ...

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