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Undergraduate Quantum Chemistry Jussi Eloranta (jmeloranta

QUANTUM CHEMISTRY • In principle, solve Schrödinger Equation • Not possible for many-electron atoms or molecules due to many-body problem ... • "Closest to H-atom solutions" • Required integrals don't have closed form • Gaussian functions: $\exp(-\frac{1}{2} r^2)$

AN INTRODUCTION TO QUANTUM CHEMISTRY

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