Search for Molecules in Magnetic Fields

Deutscher Akademischer Austauschdienst
German Academic Exchange Service

HUMBOLDT-UNIVERSITÄT ZU BERLIN

Molecules in strong Magnetic Fields show Unconventional Binding

Why Multiresolution-Analysis?

	MRA	LCAO
- BSSE error free	☺	☹
- Gauge Invariance		
- Accessing B > 2.5 a.u.		

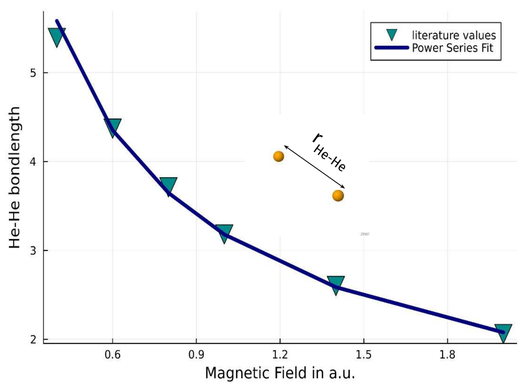
Method

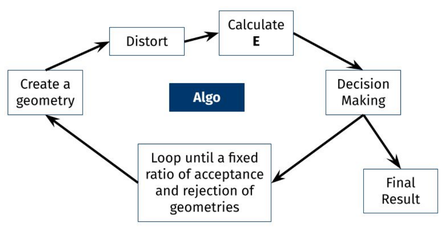
> For larger B values, no Perturbation treatment

$$\hat{H} = \hat{T} - \frac{1}{2}\mathbf{B}\cdot(\mathbf{r}\times\mathbf{p}) + \frac{1}{8}(B^2r^2 - (\mathbf{B}\cdot\mathbf{r})^2) + \hat{V}$$

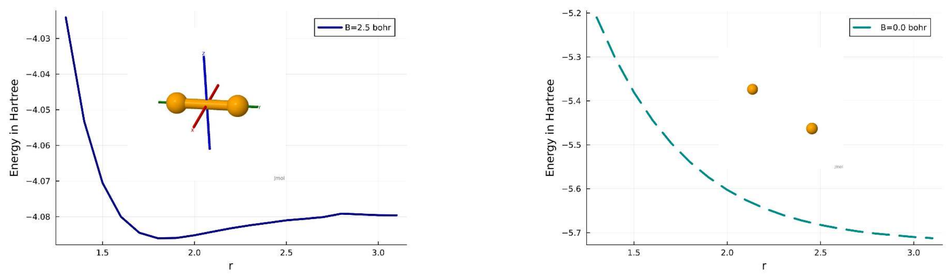
Zeeman Term — Diamagnetic Term

> Power Series Fit used to construct the initial structures for Monte-Carlo Metropolis sampling





What?



He_2 in **B**=2.5B_0 (left-bonded) and 0.0B_0 (right-dissociated) and Z-axis is **B**

Where?

NASA's James Webb Space Telescope revealing details of the Southern Ring planetary nebula

Why?

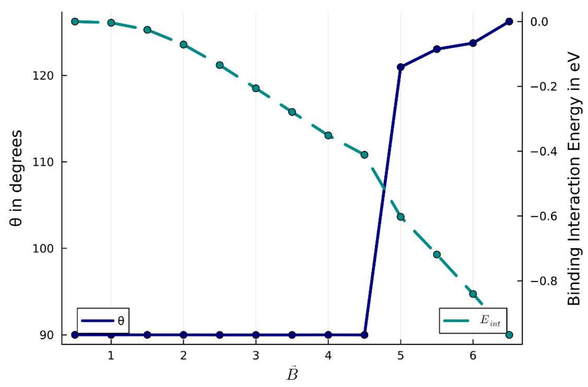
> Landau Quantization for free electron in **B**

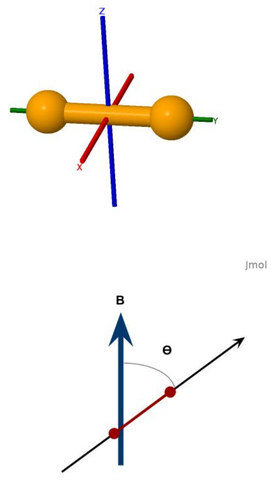
> Paramagnetic Perpendicular Bonding Mechanism

> Change in MO energy levels in presence of **B** in open shell molecules

Results So Far . . .

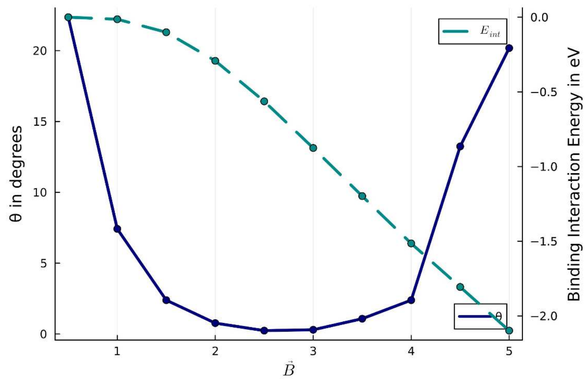
Helium Dimer (He_2)

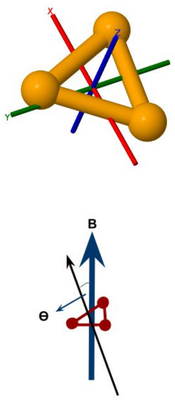




Binding Interaction Energy = E_{dimer} - (2.0 * $E_{monomer}$)

Helium Trimer (He_3)





Binding Interaction Energy = E_{trimer} - (3.0 * $E_{monomer}$)

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⚠ **Unpublished Results, for references related to this poster and contact information scan the QR-Code in the left.**