



## UPEI SEMINAR 2024

### CLIMBING DOWN THE ORDER OF PURITY



Kyle R. Bryenton  
Dalhousie Department of Physics & Atmospheric Science  
August 5, 2024

## WHO AM I?

<b>Academic Diploma</b> – Bluefield High School	2009 - 2011
<b>Bachelor of Science</b> – University of Prince Edward Island Double Major Physics (Hons. & Co-op) and Mathematics Thesis: <i>Darboux-Crum Transformations, SUSY QM, and the Eigenvalue Problem</i> Supervisors: Dr. Nasser Saad, Dr. Sheldon Opps	2011 - 2016
<b>Master of Science in Physics</b> – University of Guelph Guelph-Waterloo Physics Institute (Condensed Matter Physics / Quantum Materials) Thesis: <i>Optical Properties of the <math>\alpha</math>-T<sub>3</sub> Semi-Dirac Model</i> Supervisor: Dr. Elisabeth Nicol	2016 - 2018
<b>Research Fellow</b> – University of Prince Edward Island PI: Dr. Nasser Saad	2019
<b>AARMS Summer School</b> – University of Prince Edward Island Instructors: Dr. James Yorke & Dr. Mourad Ismail	2019
<b>Doctor of Philosophy - Ph.D Candidate, Physics</b> – Dalhousie University Department of Physics & Atmospheric Science (Chemical Physics / Density-Functional Theory) Thesis: <i>Improved Calculation of XDM Dispersion Forces, with Application to Surfaces and Interfaces</i> Supervisor: Dr. Erin Johnson	2020 - present

# PART 1: AN INTRODUCTION TO ELECTRONIC STRUCTURE

## Electronic-Structure Theory

The Schrödinger Equation

Electronic Structure Theory

Atomic Forces and Geometry Optimization

## Dispersion in Density-Functional Theory

What is Dispersion?

The London Dispersion Formula

Post-SCF Dispersion Corrections

## My Ph.D. Projects

Completed Projects

Works in Progress

## Electronic-Structure Theory

The Schrödinger Equation

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Atomic Forces and Geometry Optimization

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## My Ph.D. Projects

## EIGENVALUE EQUATIONS AND THE SCHRÖDINGER EQUATION

We begin our discussion with the Time-Independent Schrödinger Equation

$$\hat{H}\psi_n(x) = \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi_n(x) = E_n \psi_n(x)$$

This is called an eigenvalue problem, and the goal is to find both functions ( $\psi_n$ ) and corresponding eigenvalues ( $E_n$ ) which satisfy it.

### Find the eigenvalues and eigenfunctions of the momentum operator, $\hat{p}$ .

The momentum operator,  $\hat{p}$ , is given by

$$\hat{p} = \frac{\hbar}{i} \frac{d}{dx},$$

then we can assume an eigenfunction of the form  $\psi(x) = Ae^{ik(x-a)}$ , so

$$\begin{aligned}\hat{p}\psi(x) &= \left[ \frac{\hbar}{i} \frac{d}{dx} \right] \left[ Ae^{ik(x-a)} \right] \\ &= \frac{\hbar}{i} (ik) Ae^{ik(x-a)} \\ &= \hbar k \psi(x)\end{aligned}$$

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## OBSERVABLES AND EXPECTATION VALUES

We solve Schrödinger equation to determine the wavefunction,  $\psi$ . This lets us compute the expected values of “observables” of interest (e.g. position, momentum, energy, etc...).

**What is the electron's average distance from the nuclei for the hydrogen 1s orbital?**

$$\begin{aligned}\langle r \rangle &= \langle \psi(r) | r | \psi(r) \rangle \\&= \iiint \psi(r)^* r \psi(r) \cdot r^2 \sin(\theta) dr d\theta d\phi \\&= \iiint \left( \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} \right) r \left( \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} \right) r^2 \sin(\theta) dr d\theta d\phi \\&= 4\pi \left( \frac{1}{\pi a_0^3} \right) \int_0^\infty e^{-2r/a_0} r^3 dr \\&= \frac{4}{a_0^3} \left[ \frac{3a_0^4}{8} \right] \\&= \frac{3}{2} a_0\end{aligned}$$

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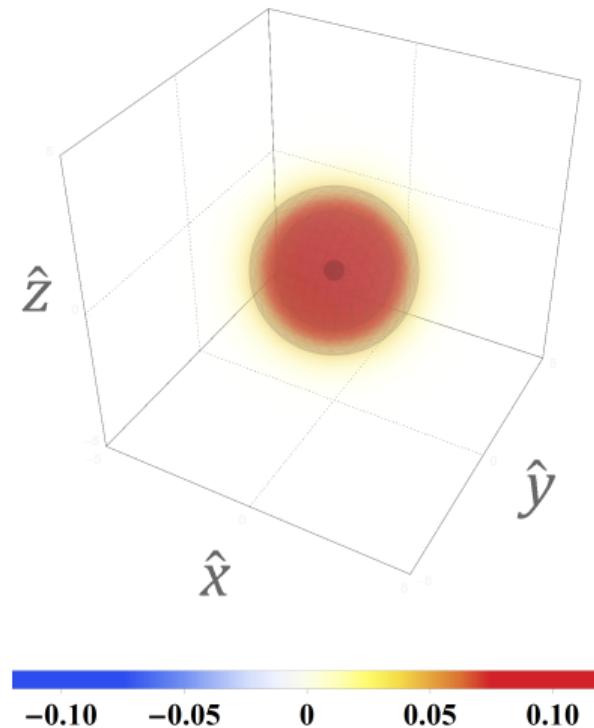
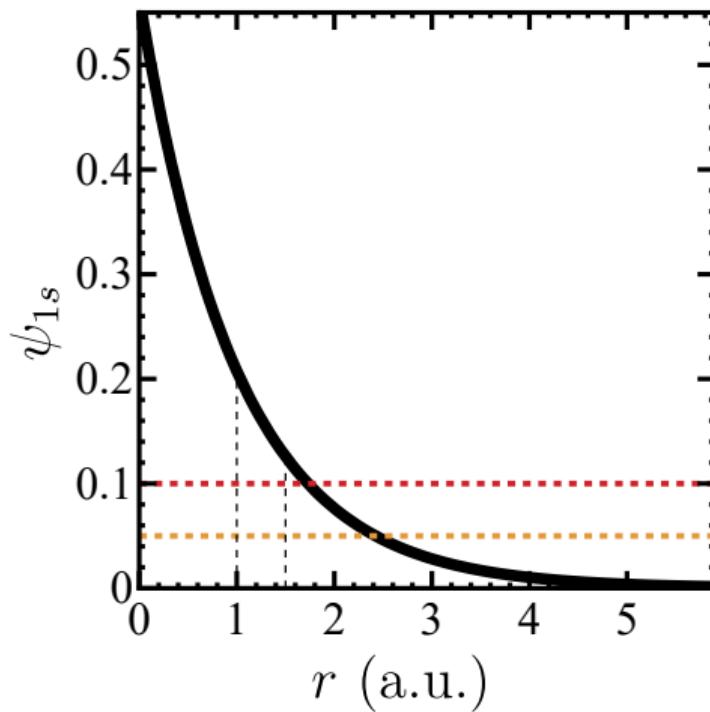
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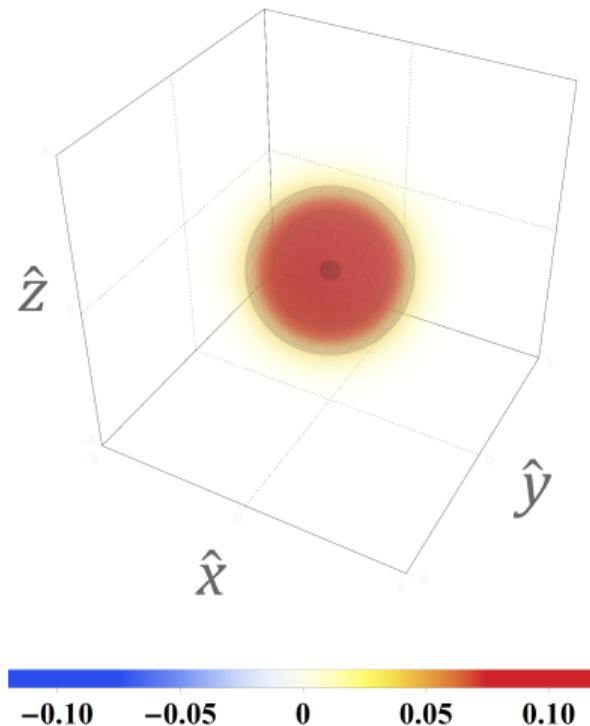
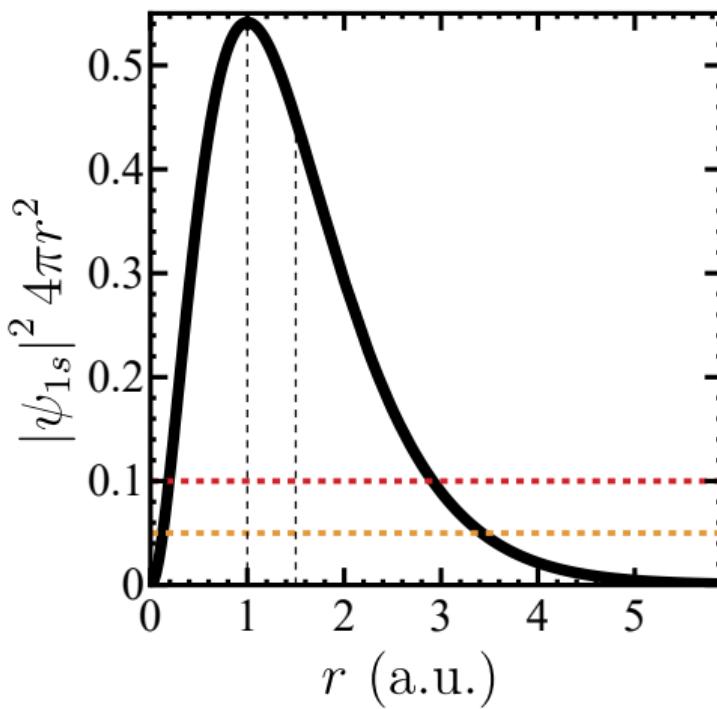
## How Do WE INTERPRET THIS?

The Bohr radius,  $a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$ , is equal to the most probable distance between the nucleus and the electron in a hydrogen atom in its ground state.



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## WAVEFUNCTION THEORY

For a general quantum system, the Hamiltonian is given by

$$\hat{H} = -\frac{1}{2} \sum_i \nabla_i^2 - \sum_{i,A} \frac{Z_A}{|\mathbf{r}_i - \mathbf{r}_A|} + \sum_{i < j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|},$$

in atomic units,  $\hbar = e = a_0 = m_e = 1$ .

However, this has severe limitations. Wavefunction methods are prohibitively costly for all but a few atoms with a dozen or fewer electrons. If we want to model any quantum systems of interest, we need to reformulate.

Instead of dealing with  $N$  electrons, we could write everything in terms of the “electron density” instead,

$$\rho(\mathbf{r}) = \sum_{i=1}^N |\psi_i(\mathbf{r})|^2$$

for  $N$  electrons occupying orbitals  $\psi_i(\mathbf{r})$ . This reduces the dimensionality of our problem from  $3N$  to just 3.

## HOHENBERG-KOHN-SHAM DFT: THE ELECTRONIC-STRUCTURE MULTI-TOOL

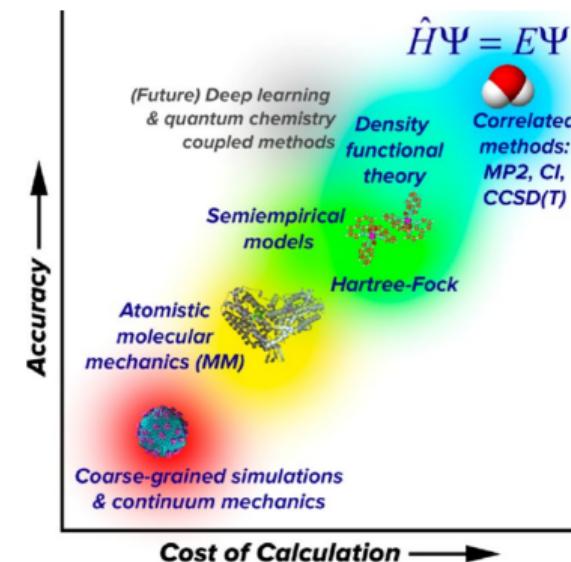
Density-functional theory (DFT) has proven to be one of the most accurate ways of calculating the electronic structure of molecules and solids while maintaining sufficiently low computational requirements.

The  $N$ -electron problem is greatly simplified by writing the total energy,

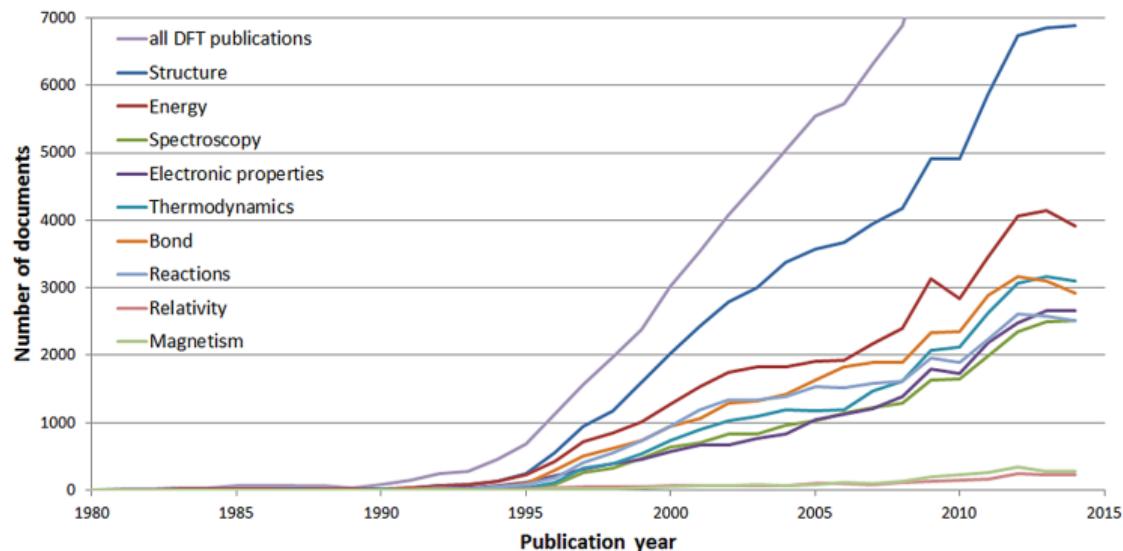
$$E[\rho] = T_s[\rho] + \int v_{\text{ext}}\rho(\mathbf{r})d\mathbf{r} + E_{\text{H}}[\rho] + E_{\text{xc}}[\rho],$$

as a functional of the electron density,  $\rho(\mathbf{r})$ . Forces are calculated via the Hellmann-Feynman theorem

$$\mathbf{F}_r = - \left\langle \frac{\partial \hat{H}}{\partial \mathbf{r}} \right\rangle = - \frac{\partial E}{\partial \mathbf{r}}$$



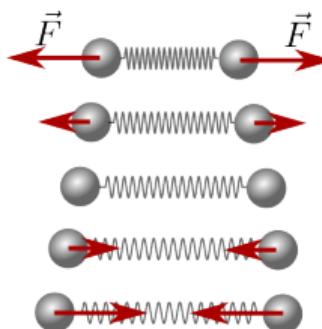
## DFT PUBLICATIONS



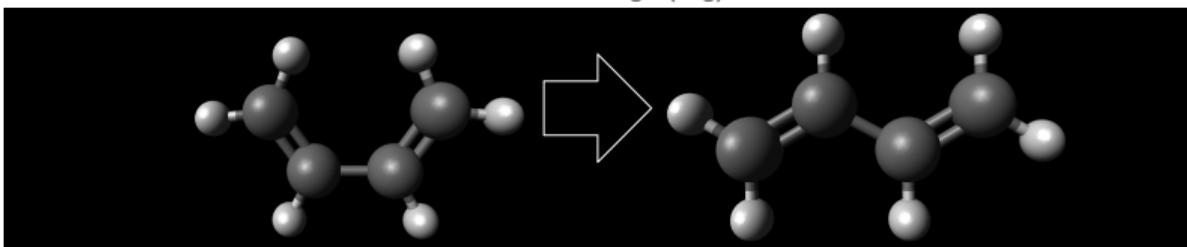
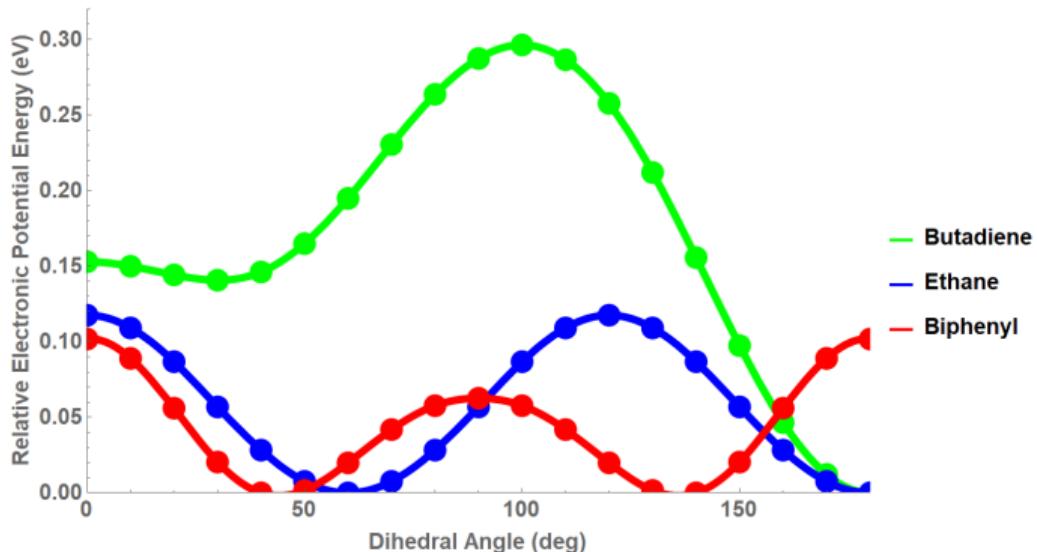
- In 2019, there were almost 15,000 confirmed DFT publications
- Very likely, more than 50,000 papers each year publish results of Kohn-Sham DFT
- In the top 10 most cited papers of all time, #7 and #8 are DFT papers
- One of these was published by Prof. Axel Becke, with almost 100,000 citations

## FORCE CALCULATIONS

- Electronic-structure theory software has a process called a geometry optimization.
- The forces on each atom are calculated in each geometry optimization step.
- The atom positions will be adjusted in the direction of the largest gradient.
- Once the atoms are moving sufficiently small within each step, they're said to be "relaxed".
- The system will adjust itself until it settles into a minimum in the potential energy surface.

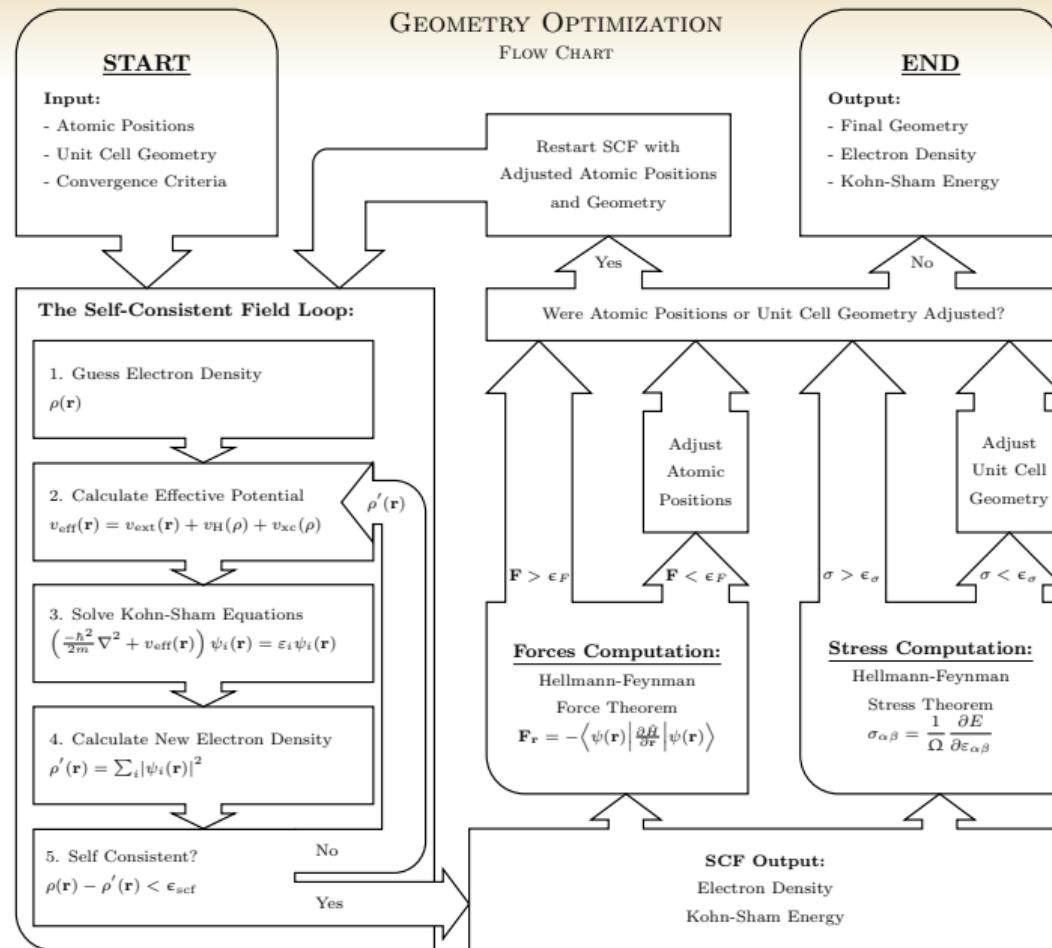


## POTENTIAL ENERGY SURFACES



# GEOMETRY OPTIMIZATION OF TRANS-OMETHOXYPHENOL

Relaxed Energy: 67.7598 kJ/mol



## Electronic-Structure Theory

## Dispersion in Density-Functional Theory

What is Dispersion?

The London Dispersion Formula

Post-SCF Dispersion Corrections

## My Ph.D. Projects

## WHAT IS DISPERSION?

London dispersion is a weak, attractive, intermolecular force.

It is considered a long-range correlation effect, caused by instantaneous dipole moments between neighbouring atoms.

Properties Determined by Dispersion:

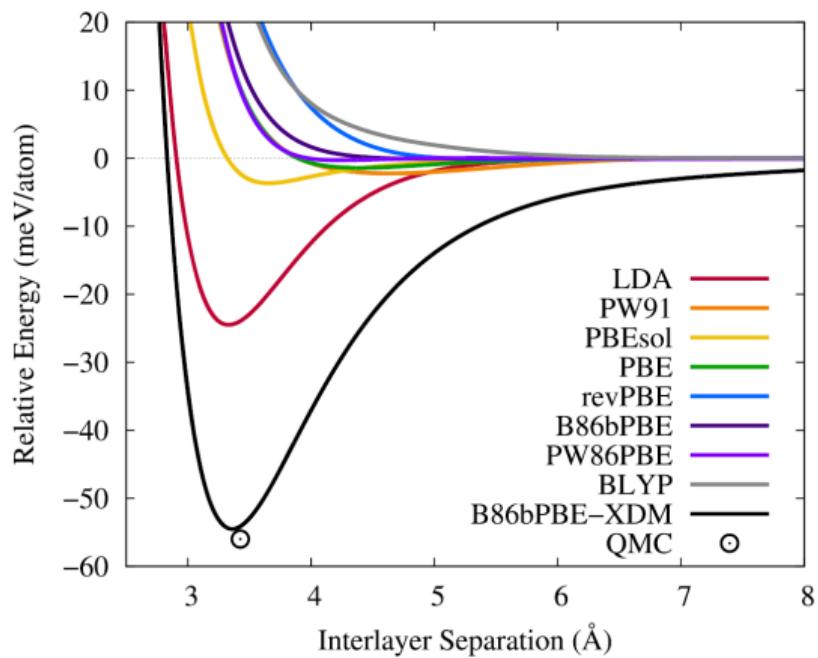
- Adhesion
- Friction
- Surface adsorption
- Phase-change conditions
- Packing in molecular crystals
- Shapes of biomolecules
- Stability of supramolecular complexes



Scamper the Gecko

## DISPERSION IN DFT

EXAMPLE: SEPARATING GRAPHITE LAYERS



## THE LONDON DISPERSION FORMULA

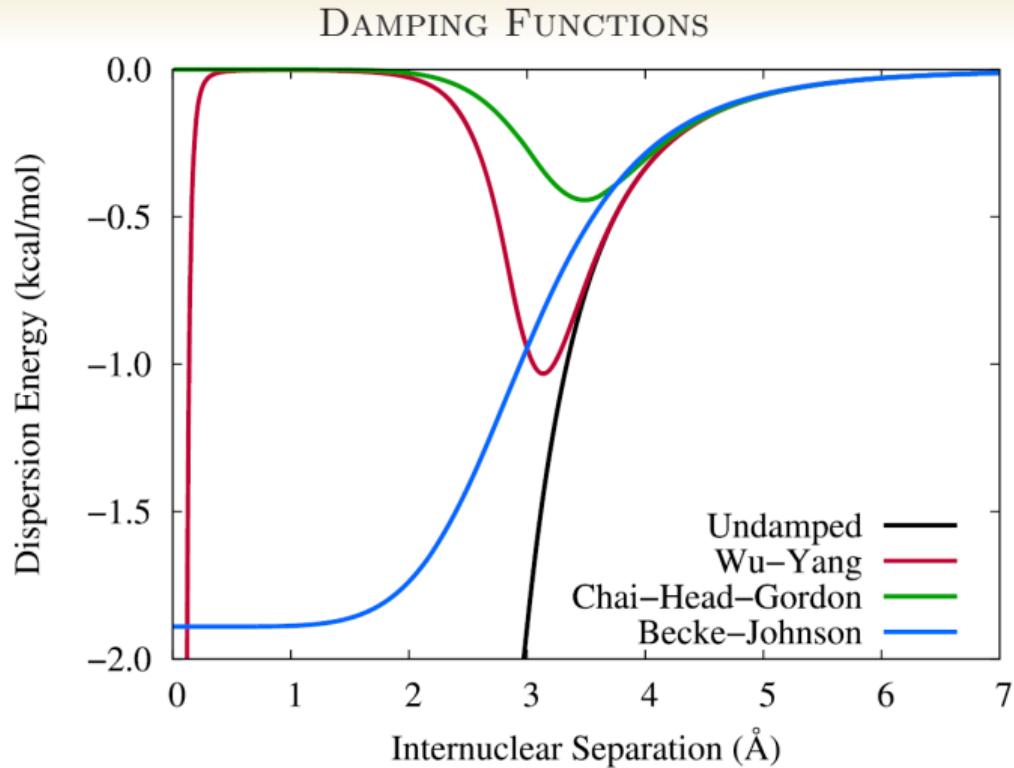
The dispersion energy can be derived using perturbation theory, and it's written as a pairwise sum over all atoms in the system,

$$E_{\text{Disp}}^{(2)} = - \sum_{i < j} \left[ \frac{C_{6,ij}}{R_{ij}^6} + \frac{C_{8,ij}}{R_{ij}^8} + \frac{C_{10,ij}}{R_{ij}^{10}} + \dots \right].$$

Atomic many-body effects refer to terms in the perturbation-theory expansion that involve more than two atoms, the leading order term is called the Axilrod-Teller-Muto (ATM) 3-body term,

$$E_{\text{Disp}}^{(3)} = \sum_{i < j < k} \frac{C_{9,ijk} [3 \cos(\theta_i) \cos(\theta_j) \cos(\theta_k) + 1]}{R_{ij}^3 R_{jk}^3 R_{ki}^3}.$$

Electronic many-body effects refer to the sensitivity of the  $C_n$  coefficients to their chemical environment, and are far more important than atomic many-body effects.



## THE TKATCHENKO-SCHEFFLER (TS) MODEL

The Tkatchenko-Scheffler (TS) model only considers dipole-dipole interactions and determines  $C_{6,ii}$ ,  $\alpha_i^0$ , and  $R_i^0$  from their free-atom reference values using effective volumes.

$$E_{\text{TS}} = - \sum_{i < j} f_{\text{TS}}^{\text{WY}}(R_{ij}) \frac{C_{6,ij}^{\text{TS}}}{R_{ij}^6}$$

## THE EXCHANGE-HOLE DIPOLE MOMENT (XDM) MODEL

The exchange-hole dipole moment (XDM) model includes higher-order terms and determines  $C_{6,ii}$  and  $R_{\text{vdW}}$  via multipole moment integrals. The polarizability is determined from free-atom reference values using effective volumes.

$$E_{\text{XDM}} = - \sum_{i < j} \sum_{n=6,8,10} f_n^{\text{BJ}}(R_{ij}) \frac{C_{n,ij}^{\text{XDM}}}{R_{ij}^n}$$

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Dispersion in Density-Functional Theory  
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My Ph.D. Projects  
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## Electronic-Structure Theory

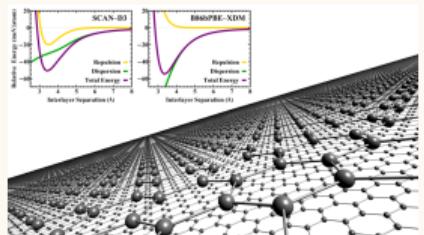
## Dispersion in Density-Functional Theory

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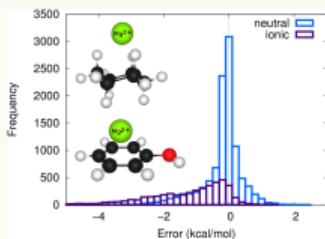
Works in Progress

## Requirements for an Accurate Disp.-Corr. Functional



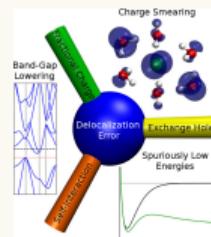
A. J. A. Price, K. R. Bryenton, & E. R. Johnson, *J. Chem. Phys.* **154**, 230902 (2021).  
doi: 10.1063/5.0050993

## Comparison of DFT Disp. Corrections on DES15K



C. J. Nickerson, K. R. Bryenton, A. J. Price, & E. R. Johnson, *J. Phys. Chem. A* **127**(41), 8712-8722 (2023) doi: 10.1021/acs.jpca.3c04332

## Delocalization Error: Greatest Outstanding Challenge



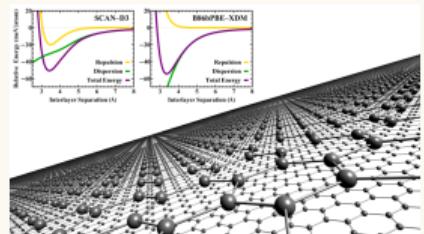
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## Many-Body Dispersion and the Sensitivity of SCS



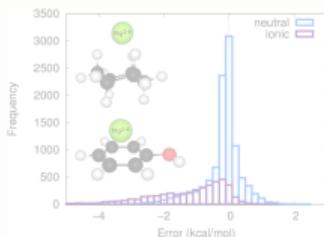
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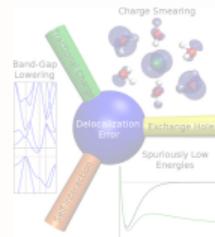
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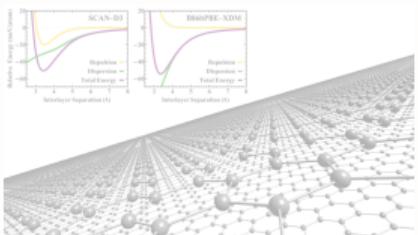
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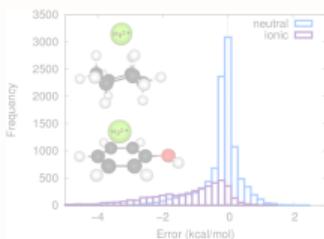
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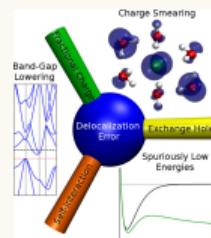
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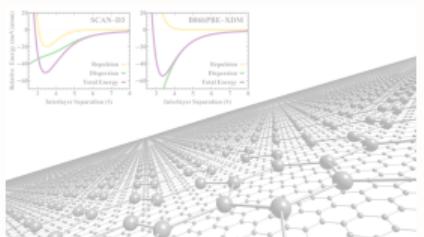
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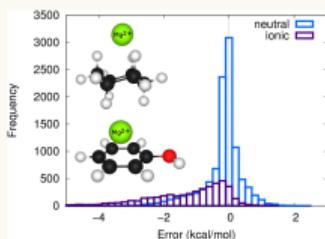
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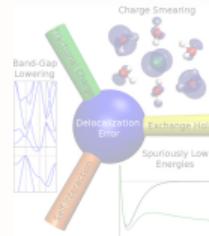
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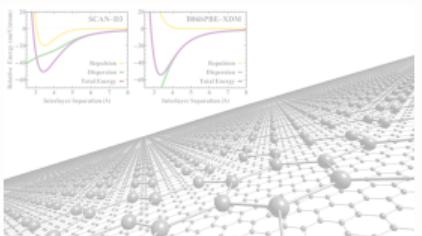
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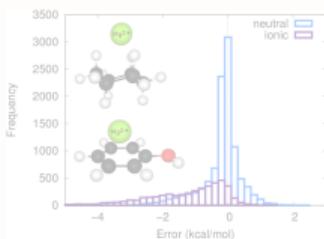
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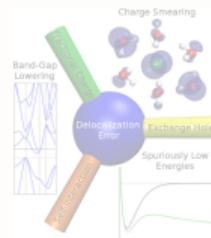
A. J. A. Price, K. R. Bryenton, & E. R. Johnson, *J. Chem. Phys.* **154**, 230902 (2021).  
doi: 10.1063/5.0050993

## Comparison of DFT Disp. Corrections on DES15K



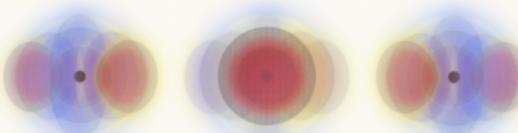
C. J. Nickerson, K. R. Bryenton, A. J. Price, & E. R. Johnson, *J. Phys. Chem. A* **127**(41), 8712-8722 (2023) doi: 10.1021/acs.jpca.3c04332

## Delocalization Error: Greatest Outstanding Challenge



K. R. Bryenton, A. A. Adeleke, S. G. Dale, & E. R. Johnson, *WIREs Comp. Mol. Sci.* **13**, e1631 (2023). doi: 10.1002/wcms.1631

## Many-Body Dispersion and the Sensitivity of SCS



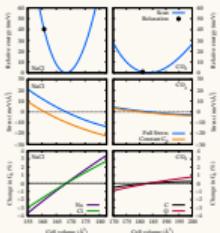
K. R. Bryenton & E. R. Johnson, *J. Chem. Phys.* **158**, 204110 (2023). doi: 10.1063/5.0142465

## Density-Based London Dispersion Corr. to DFT



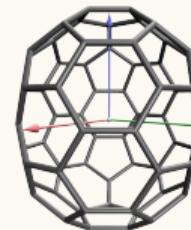
A. Tkatchenko, A. Ambrosetti, **K. R. Bryenton**, E. R. Johnson, et al., Manuscript in Preparation (2024).

## Improvement to XDM Dispersion Forces



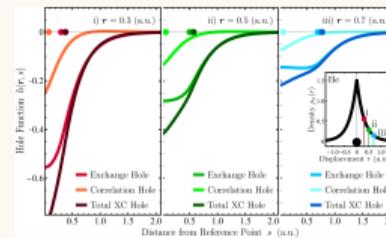
**K. R. Bryenton**, A. Otero-da-la-Roza, & E. R. Johnson, Eternally Stuck on a Bug (2024).

## High accuracy for disp.-bound systems: Ne@C70



K. Panchagnula, D. Graf, E. R. Johnson, **K. R. Bryenton**, A. J. W. Thom, Manuscript in Preparation (2024).

## XCDM: Exchange-correlation-hole Dipole Moment



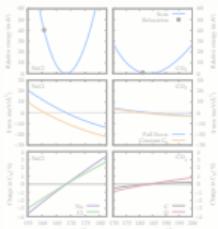
**K. R. Bryenton**, & E. R. Johnson, Manuscript in Preparation (2024).

## Density-Based London Dispersion Corr. to DFT



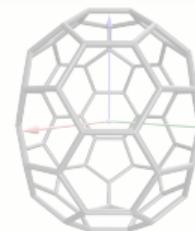
A. Tkatchenko, A. Ambrosetti, K. R. Bryenton, E. R. Johnson, et al., Manuscript in Preparation (2024).

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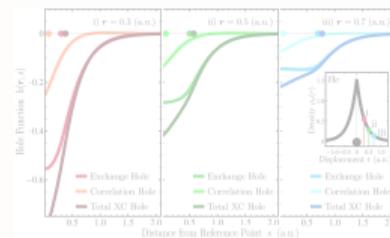
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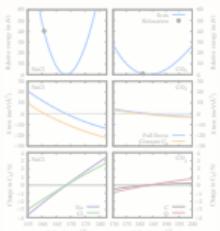
K. R. Bryenton, & E. R. Johnson, Manuscript in Preparation (2024).

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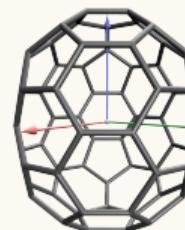
A. Tkatchenko, A. Ambrosetti, K. R. Bryenton, E. R. Johnson, et al., Manuscript in Preparation (2024).

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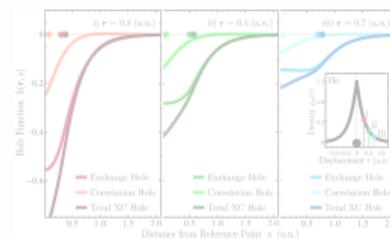
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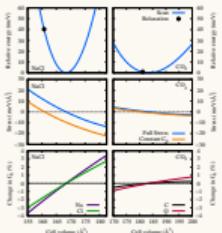
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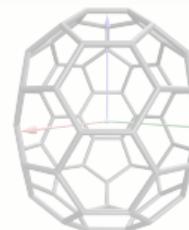
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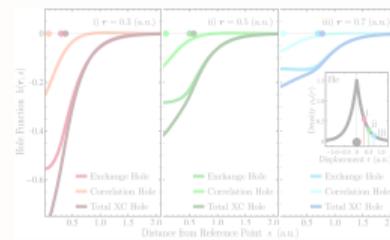
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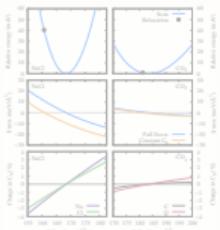
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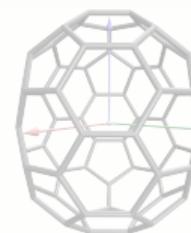
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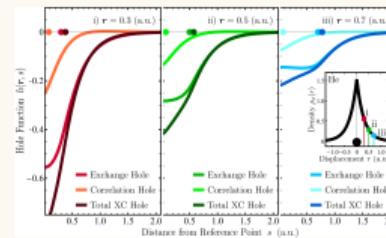
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K. R. Bryenton, & E. R. Johnson, Manuscript in Preparation (2024).

## PART 2: ADDING CORRELATION TO THE EXCHANGE-HOLE DIPOLE MOMENT (XDM) MODEL

### Introduction

What is Dispersion?

XDM: The Exchange-hole Dipole Moment Model

Motivation

### XCDM Implementation

Short-Range Dynamical Correlation Models

Plots of the Exchange-Correlation Hole

### Results

Benchmark Sets

Qualitative Results and Observations

### Conclusions

## Introduction

What is Dispersion?

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## WHAT IS DISPERSION?

London dispersion is a weak, attractive, intermolecular force.

It is considered a long-range correlation effect, caused by instantaneous dipole moments between neighbouring atoms.

Properties Determined by Dispersion:

- Adhesion
- Friction
- Surface adsorption
- Phase-change conditions
- Packing in molecular crystals
- Shapes of biomolecules
- Stability of supramolecular complexes



Scamper the Gecko

## THE XDM MODEL

The exchange-hole dipole moment (XDM) model calculates the dispersion energy via a pairwise sum over all atoms,

$$E_{\text{XDM}} = - \sum_{j < i} \sum_{n=6,8,10} f_n^{\text{BJ}}(R_{ij}) \frac{C_{n,ij}}{R_{ij}^n}.$$

Here,  $f_n^{\text{BJ}}(R_{ij})$  is the Becke-Johnson damping function to prevent convergence at small interatomic separations,  $R_{ij}$ . The XDM model calculates the dispersion coefficients,  $C_n$ , using exchange-hole dipole moments,

$$d_{X\sigma}(\mathbf{r}) = \left[ \int h_{X\sigma}(\mathbf{r}, \mathbf{s}) s d\mathbf{s} \right] - \mathbf{r},$$

which are obtained by integrating the exchange hole,  $h_{X\sigma}$ , over its reference point,  $\mathbf{s}$ .

These exchange-hole dipole moments are used along with Hirshfeld weights,  $w_i$ , and the electron density,  $\rho_\sigma$ , to compute the multipole moment integrals,

$$\langle M_\ell^2 \rangle = \sum_{\sigma} \int w_i(\mathbf{r}) \rho_\sigma(\mathbf{r}) \left[ r^\ell - (r - d_{\times\sigma})^\ell \right]^2 d\mathbf{r}.$$

These are then combined with atom-in-molecule polarizabilities,  $\alpha_i$ , to solve for the heteroatomic dispersion coefficients,

$$C_{6,ij}^{\text{XDM}} = \frac{\alpha_i \alpha_j \langle M_1^2 \rangle_i \langle M_1^2 \rangle_j}{\alpha_i \langle M_1^2 \rangle_j + \alpha_j \langle M_1^2 \rangle_i}$$

$$C_{8,ij}^{\text{XDM}} = \frac{3}{2} \frac{\alpha_i \alpha_j \left( \langle M_1^2 \rangle_i \langle M_2^2 \rangle_j + \langle M_2^2 \rangle_i \langle M_1^2 \rangle_j \right)}{\alpha_i \langle M_1^2 \rangle_j + \alpha_j \langle M_1^2 \rangle_i}$$

$$C_{10,ij}^{\text{XDM}} = 2 \frac{\alpha_i \alpha_j \left( \langle M_1^2 \rangle_i \langle M_3^2 \rangle_j + \langle M_3^2 \rangle_i \langle M_1^2 \rangle_j \right)}{\alpha_i \langle M_1^2 \rangle_j + \alpha_j \langle M_1^2 \rangle_i} + \frac{21}{5} \frac{\alpha_i \alpha_j \langle M_2^2 \rangle_i \langle M_2^2 \rangle_j}{\alpha_i \langle M_1^2 \rangle_j + \alpha_j \langle M_1^2 \rangle_i}.$$

## MOTIVATION

"Why does XDM only use the exchange hole and not the exchange-correlation hole?"

### REASONS:

1. The contribution from exchange dominates over correlation
2. XDM uses the BR-hole, which partially models non-dynamical correlation
3. The contribution from dynamical correlation has been shown to be small

... Though, it'd be nice to properly include dynamical correlation.

### WHAT WE'VE DONE:

1. Derived same- and opposite-spin correlation hole models
2. Integrated them into XDM in the FHI-aims code
3. Extensive Benchmarking

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## Introduction

## XCDM Implementation

- Short-Range Dynamical Correlation Models
- Plots of the Exchange-Correlation Hole

## Results

## Conclusions

## SHORT-RANGE DYNAMICAL CORRELATION MODELS

We can simply expand the hole term from the previous slide to include terms for the same- and opposite-spin dynamical correlation holes

$$d_{XC\sigma}(\mathbf{r}) = \left[ \int h_{XC}(\mathbf{r}, \mathbf{s}) s d\mathbf{s} \right] - \mathbf{r} = \left[ \int \left( h_{X\sigma}(\mathbf{r}, \mathbf{s}) + h_{C\sigma}^{\sigma\sigma}(\mathbf{r}, \mathbf{s}) + h_{C\sigma}^{\alpha\beta}(\mathbf{r}, \mathbf{s}) \right) s d\mathbf{s} \right] - \mathbf{r}.$$

$h_{X\sigma}$  is currently captured via the framework of the BR hole, which we can leverage to capture  $d_{XC\sigma}$ . Becke proposed analogous models for the same- and opposite-spin dynamical correlation holes of the form

$$h_{C\sigma}^{\sigma\sigma}(\mathbf{r}, \mathbf{s}) = \frac{s^2 (s - z_{\sigma\sigma}) D_\sigma(\mathbf{r})}{3(2 + z_{\sigma\sigma})} f(\gamma_{\sigma\sigma} s) \quad h_{C\sigma}^{\alpha\beta}(\mathbf{r}, \mathbf{s}) = \frac{(s - z_{\alpha\beta}) \rho_\sigma(\mathbf{r})}{1 + z_{\alpha\beta}} f(\gamma_{\alpha\beta} s),$$

where  $z$  is the spin-dependent correlation length,  $D_\sigma = \tau_\sigma - \tau_\sigma^W$  is the difference between the exact kinetic-energy density and the von Weizsäker approximation, and  $f(\gamma s)$  is a function that serves to normalize these correlation holes to 0 electrons.

Becke proposed three forms for the normalization function

$$f(\gamma s) = \begin{cases} \operatorname{sech}(\gamma s) \\ (1 + \gamma s) e^{-\gamma s} \\ e^{-(\gamma s)^2} \end{cases} .$$

Spherical integration of these correlation hole models lead to the following expressions for the same- and opposite-spin correlation hole dipole moments,

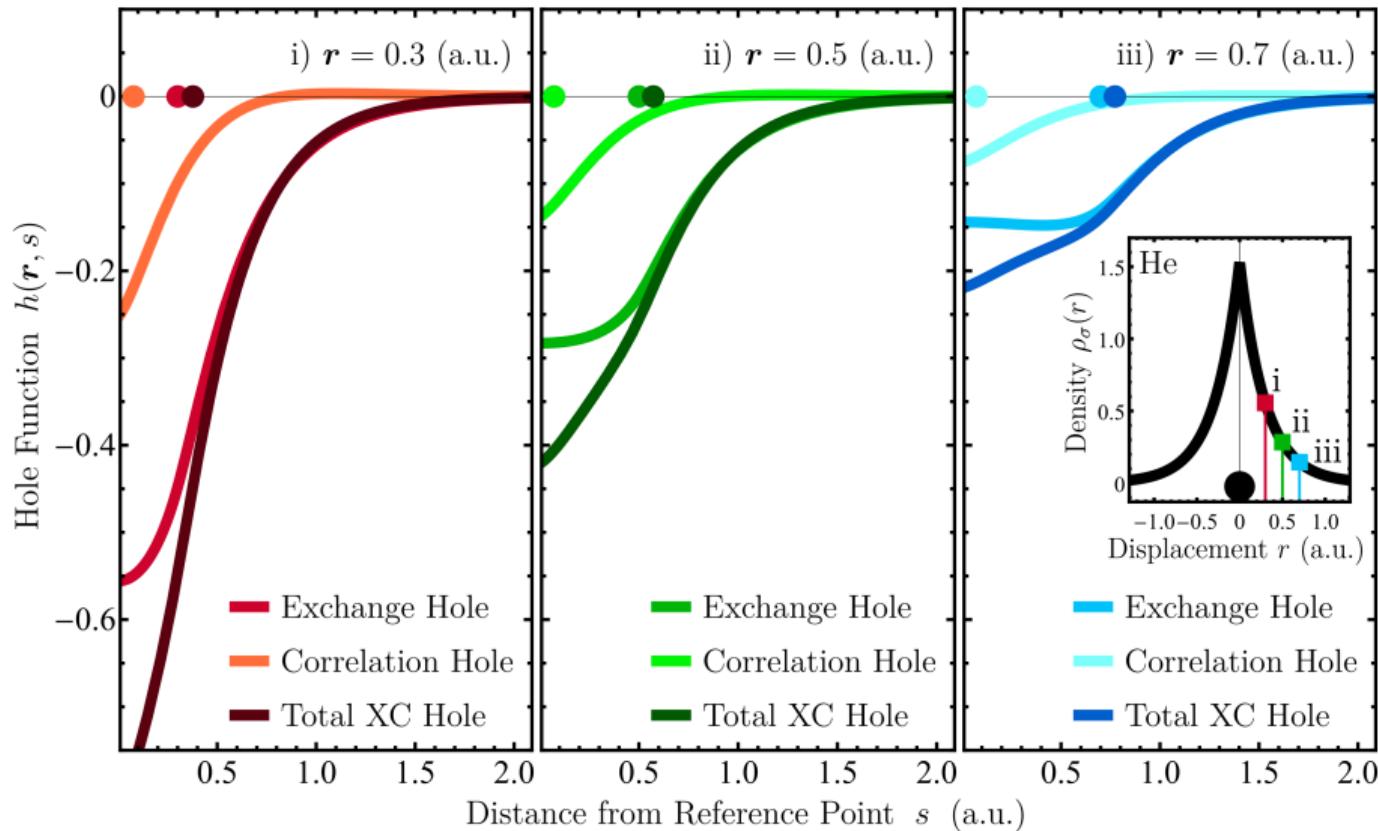
$$d_{C\sigma}^{\sigma\sigma}(\mathbf{r}) = \left[ \int h_C^{\sigma\sigma}(\mathbf{r}, \mathbf{s}) s d\mathbf{s} \right] - \mathbf{r} = \frac{c_{\sigma\sigma} z_{\sigma\sigma}^7}{2 + z_{\sigma\sigma}} D_\sigma(\mathbf{r}) - \mathbf{r} ,$$

$$d_{C\sigma}^{\alpha\beta}(\mathbf{r}) = \left[ \int h_C^{\alpha\beta}(\mathbf{r}, \mathbf{s}) s d\mathbf{s} \right] - \mathbf{r} = \frac{c_{\alpha\beta} z_{\alpha\beta}^5}{1 + z_{\alpha\beta}} \rho_\sigma(\mathbf{r}) - \mathbf{r} .$$

Here,  $c_{\sigma\sigma} \approx 0.02$  and  $c_{\alpha\beta} \approx 0.6$ ; the exact value depends on the chosen form of  $f(\gamma s)$ . Now, our description of the exchange-correlation-hole dipole moment is complete:

$$d_{XC\sigma}(\mathbf{r}) = \left[ \int h_{X\sigma}(\mathbf{r}, \mathbf{s}) s d\mathbf{s} + \frac{c_{\sigma\sigma} z_{\sigma\sigma}^7}{2 + z_{\sigma\sigma}} D_\sigma(\mathbf{r}) + \frac{c_{\alpha\beta} z_{\alpha\beta}^5}{1 + z_{\alpha\beta}} \rho_\sigma(\mathbf{r}) \right] - \mathbf{r} .$$

## PLOTS OF THE EXCHANGE-CORRELATION HOLE



## Introduction

## XCDM Implementation

## Results

Benchmark Sets

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## BENCHMARKING

### Basis Sets:

- Light
- LightDense
- Intermediate
- Tight

### Functionals:

- B86bPBE
- B86bPBE-25
- B86bPBE-50
- PBE
- PBE0
- PBE-50
- HSE06

XCDM is currently implemented into a private version of the FHI-aims code.

### Benchmarks:

- |                  |  |
|------------------|--|
| • KB49           | – Intermolecular Complexes               |
| • MolC6          | – Molecular $C_6$ Coefficients           |
| • S22 $\times$ 5 | – Small Molecular Dimers & Non-Eq. Geoms |
| • S66 $\times$ 8 | – Small Molecular Dimers & Non-Eq. Geoms |
| • 3B-69          | – Small Molecular Trimers                |
| • Heavy28        | – Complexes with Heavy Atom Hydrides     |
| • L7             | – Large Molecular Complexes              |
| • S6L            | – Large Molecular Complexes              |
| • X23            | – Molecular Crystals                     |
| • Ice13          | – Ice Crystal Phases                     |
| • HalCrys4       | – Halogen Crystals                       |
| • LM26           | – Layered Materials                      |

## QUALITATIVE RESULTS AND OBSERVATIONS

## XCDM compared to XDM: Mean Absolute Error % Change

Benchmark	MAE Chg.	Description
KB49	↓ 1%	Intermolecular Complexes
MolC6	↓ 15%	Molecular $C_6$ Coefficients
S22×5	~	Small Molecular Dimers & Non-Eq. Geoms
S66×8	~	Small Molecular Dimers & Non-Eq. Geoms
3B-69	↓ 2%	Small Molecular Trimers
Heavy28	↓ 3%	Complexes with Heavy Atom Hydrides
L7	↓ 2%	Large Molecular Complexes
S6L	↓ 10%	Large Molecular Complexes
X23	↓ 5%	Molecular Crystals
Ice13	~	Ice Crystal Phases
HalCrys4	↑ 1%	Halogen Crystals
LM26	↑ 5%	Layered Materials

Observations:

- Our previous conjecture that dynamical correlation doesn't matter much was generally correct
- MolC6's improvement shows we're accurately modelling the physics
- XCDM typically captures an additional 0.02-0.10 kcal/mol binding energy
- If XDM overbinds, XCDM often (but not always) compounds the error

Introduction  
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XCDM Implementation  
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Results  
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Conclusions  
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## Introduction

## XCDM Implementation

## Results

## Conclusions

## KEY TAKEAWAYS

1. For small molecular systems, XDM and XCDM perform about equivalently
2. For large molecular systems or crystal structure prediction, use XCDM for increased accuracy
3. For layered materials, systems with large delocalization error, or other systems where XDM overbinds, using XCDM might worsen the error

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- Walter C. Sumner Foundation
- Government of Nova Scotia
- Dalhousie University
- Digital Research Alliance of Canada
- ACENET
- FHI-aims

# QUESTIONS?

WANT MY SLIDES?



[HTTPS://GITHUB.COM/KYLEBRYENTON/SLIDES-POSTERS](https://github.com/kylebryenton/slides-posters)

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