



PHD DEFENCE
PHYSICS-GUIDED SOLUTIONS TO DISPERSION
IN DENSITY-FUNCTIONAL THEORY



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PhD Contributions

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Introduction

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Oscillators Project

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XCDM Project

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Conclusions

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PhD Contributions

Thesis Projects

Other Projects

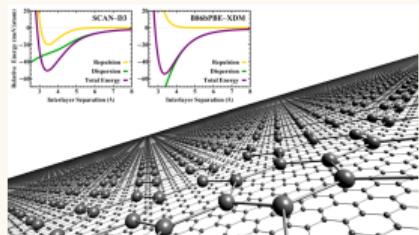
Introduction

Oscillators Project

XCDM Project

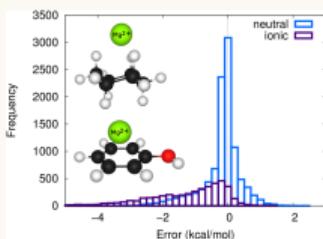
Conclusions

Requirements for an Accurate Disp.-Corr. Functional



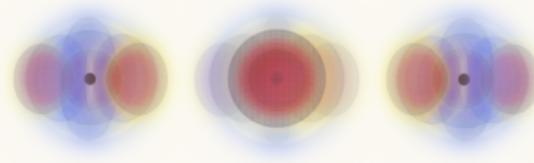
A. J. A. Price, K. R. Bryenton, & E. R. Johnson, *J. Chem. Phys.* **154**, 230902 (2021).
doi: 10.1063/5.0050993

Comparison of DFT Disp. Corrections on DES15K



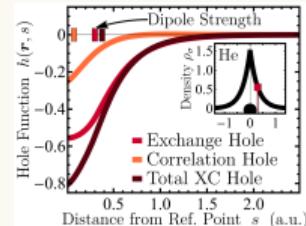
C. J. Nickerson, K. R. Bryenton, A. J. Price, & E. R. Johnson, *J. Phys. Chem. A* **127**(41), 8712-8722 (2023) doi: 10.1021/acs.jpca.3c04332

Many-Body Dispersion and the Sensitivity of SCS



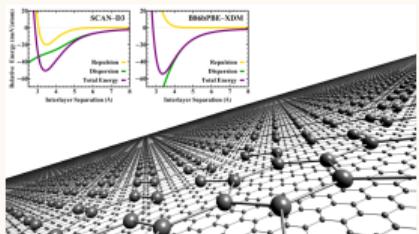
K. R. Bryenton & E. R. Johnson, *J. Chem. Phys.* **158**, 204110 (2023). doi: 10.1063/5.0142465

The Exchange-Correlation Dipole Moment Model



K. R. Bryenton, & E. R. Johnson, Submitted to: *Phys. Chem. Chem. Phys.* (2025). doi: 10.48550/arXiv.2506.02352

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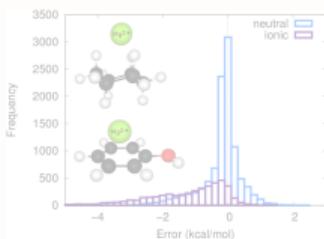
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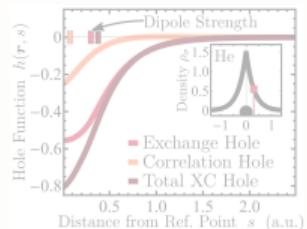
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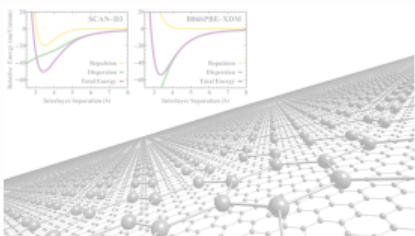
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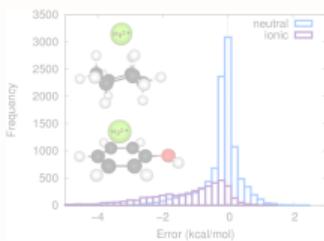
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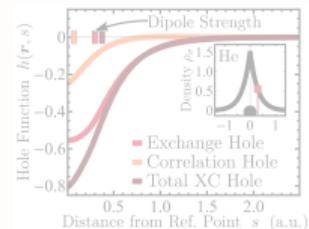
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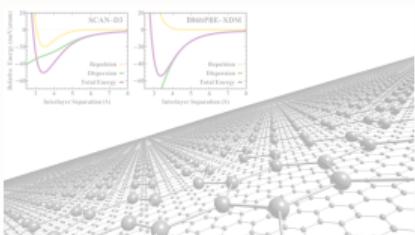
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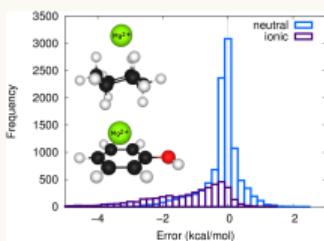
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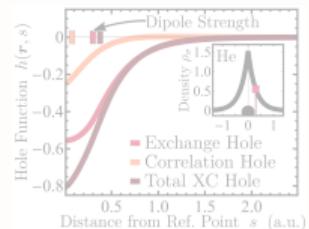
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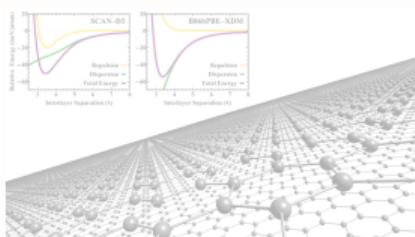
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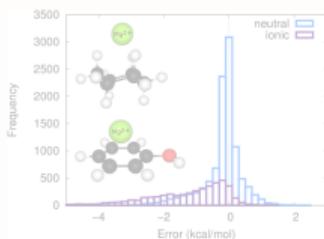
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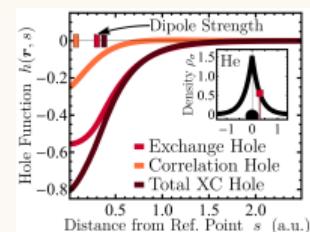
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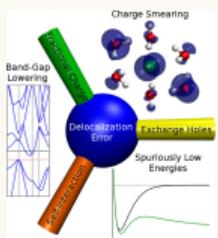


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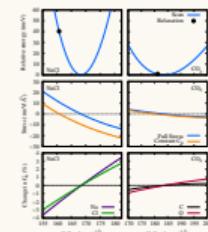
K. R. Bryenton, A. A. Adeleke, S. G. Dale, & E. R. Johnson, *WIREs Comp. Mol. Sci.* 13, e1631 (2023). doi: 10.1002/wcms.1631

Roadmap on Advancements of the FHI-aims Software



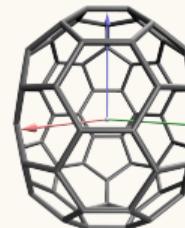
V. Blum, et al. (including: K. R. Bryenton), Submitted to: *Electron. Struct.* (2025)
doi: 10.48550/arXiv.2505.00125

Improvement of XDM Dispersion Forces



K. R. Bryenton, A. Otero-da-la-Roza, & E. R. Johnson, Project on Hold (2024).

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



K. Panchagnula D. Graf, K. R. Bryenton, E. R. Johnson, A. J. W. Thom, Manuscript in Preparation (2024). doi: 10.48550/arXiv.2503.01637

PhD Contributions
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PhD Contributions

Introduction

What is Dispersion?

Many-Body Dispersion Effects

Post-SCF Dispersion Corrections

Oscillators Project

XCDM Project

Conclusions

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

ELECTRONIC MANY-BODY EFFECTS

Refer to the responsiveness of the dispersion coefficients to changes in the atomic environment.

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

ATOMIC MANY-BODY EFFECTS

Refer to terms in the perturbation-theory expansion of the dispersion energy that involve more than two atoms. These typically contribute negligibly to the total dispersion energy.

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

THE TS MODEL

The Tkatchenko–Scheffler (TS) model only considers dipole-dipole interactions and determines $C_{6,ii}$, α_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 XDM MODEL

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

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

THE MBD@rsSCS MODEL

The many-body dispersion (MBD) model refines its coefficients through range-separated self-consistent screening (rsSCS).

$$\alpha_i^{\text{SCS}}(i\omega) = \alpha_i^{\text{TS}}(i\omega) + \alpha_i^{\text{TS}}(i\omega) \sum_{j \neq i} \mathbf{T}_{ij} \alpha_j^{\text{SCS}}(i\omega)$$

The dispersion energy is calculated through the use of the coupled fluctuating dipole model (CFDM) Hamiltonian.

$$E_{\text{MBD}} = \frac{1}{2} \sum_{i=1}^{3N} \sqrt{\lambda_i} - \frac{3}{2} \sum_{i=1}^N \omega_i^{\text{SCS}}$$

THE MBD-NL MODEL

The imprecisely named non-local (NL) MBD model uses Vydrov and Van Voorhis VV10's semi-local polarizability model, forgoing SCS, and improving performance and stability.

$$\alpha^{\text{VV}}[\rho](\mathbf{r}, i\omega) = \frac{\rho(\mathbf{r})}{\frac{4\pi}{3} + C \frac{|\nabla \rho(\mathbf{r})|^4}{\rho(\mathbf{r})^4} + \omega^2}$$

Tkatchenko *et al.*, *Phys. Rev. Lett.* **108**, 236402. (2012) doi: 10.1103/PhysRevLett.108.236402
Hermann & Tkatchenko, *Phys. Rev. Lett.* **124**, 146401. (2020) doi: 10.1103/PhysRevLett.124.146401

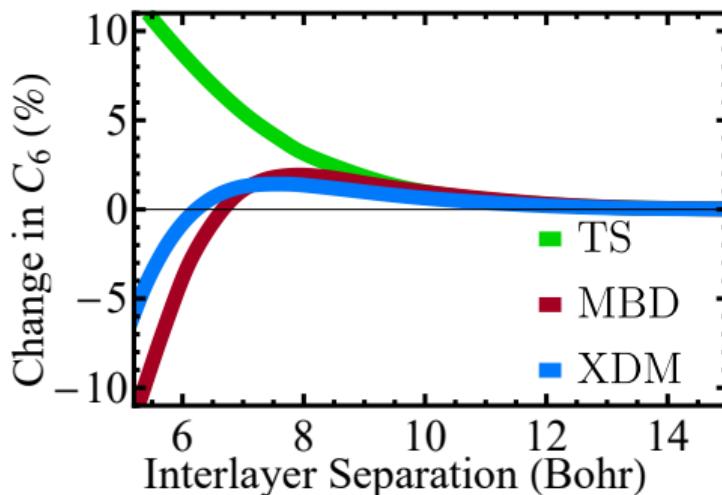
SUMMARY OF DISPERSION CORRECTIONS

α	Polarizability	SCS	Self-Consistent Screening
C_n	Dispersion Coefficients	CFDM	Coupled-Fluctuating Dipole Model
R_{vdw}	van der Waals Radius	TS	Tkatchenko–Scheffler Model
WY	Wu–Yang Damping	XDM	Exchange–Hole Dipole Moment
BJ	Becke–Johnson Damping	MBD	Many-Body Dispersion Model
VV10	Vydrov and Van Voorhis	MBD-NL	Non-Local MBD Dispersion Model

Table comparing different post-SCF dispersion corrections (Incomplete)

Disp.	Damping	C_6	$> C_6$	Empiricism	Elec.	Atom.
TS:	WY	✓	✗	α, C_6, R_{vdw}	?	✗
XDM:	BJ	✓	✓	α	?	C_9
MBD:	rsSCS	✓	?	TS@SCS	?	✓
MBD-NL:	rs	✓	?	VV10	?	✓
MBD-Free:	rsSCS	✓	?	Free@SCS	?	✓
MBD-XDM:	rsSCS	✓	?	$\alpha+SCS$?	✓

MOTIVATION: XDM vs. MBD SEPARATING GRAPHITE LAYERS



RESEARCH GOAL:

1. Compare TS, MBD, and XDM on model systems, molecular systems, and layered materials.
2. Study how each method captures many-body effects.

Adapted with permission from:

Otero-de-la-Roza *et al.*, *J. Phys. Chem. Lett.* **11**, 2298–2302. (2020) doi: 10.1021/acs.jpclett.0c00348

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Oscillators Project

The Oscallot Code

Results from Oscillator and Noble Gas Model Systems

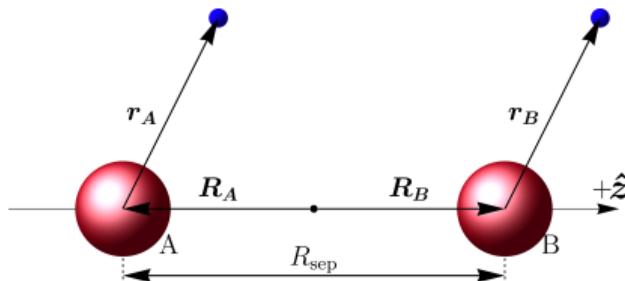
Connection with Molecular Dimers and Layered Materials

XCDM Project

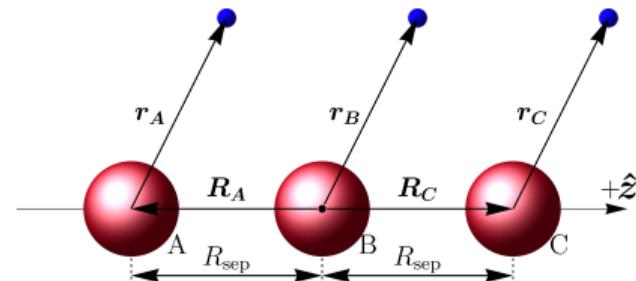
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SYSTEM GEOMETRY

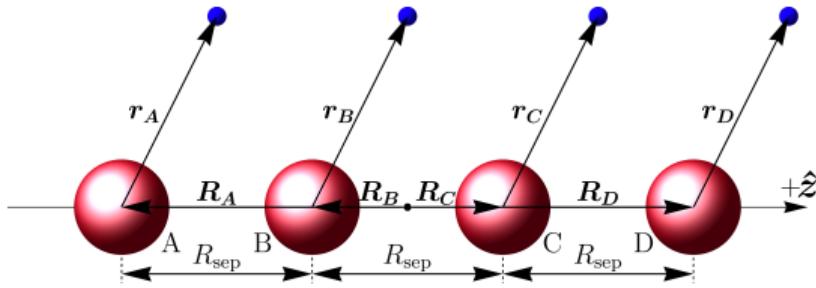
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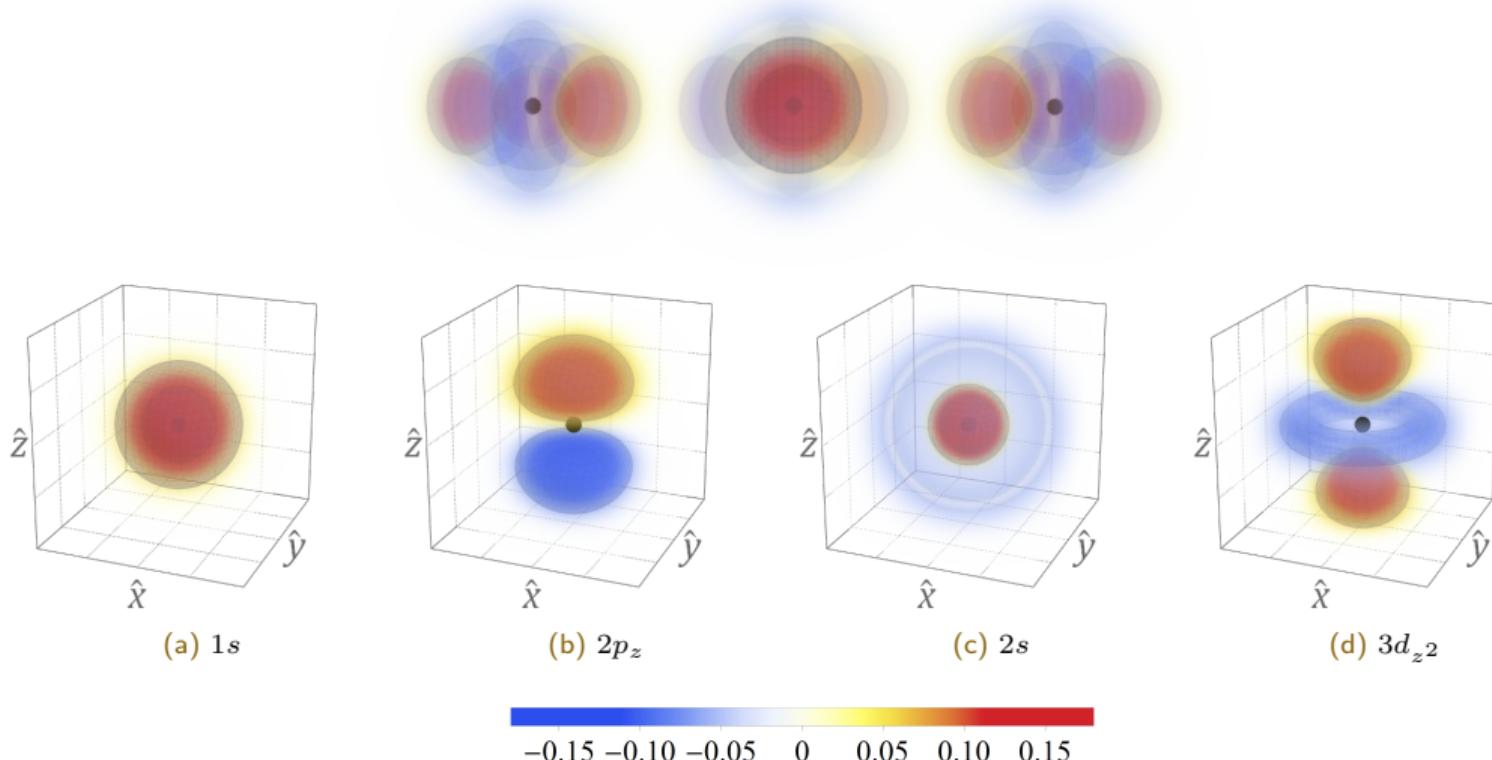
TRIMER



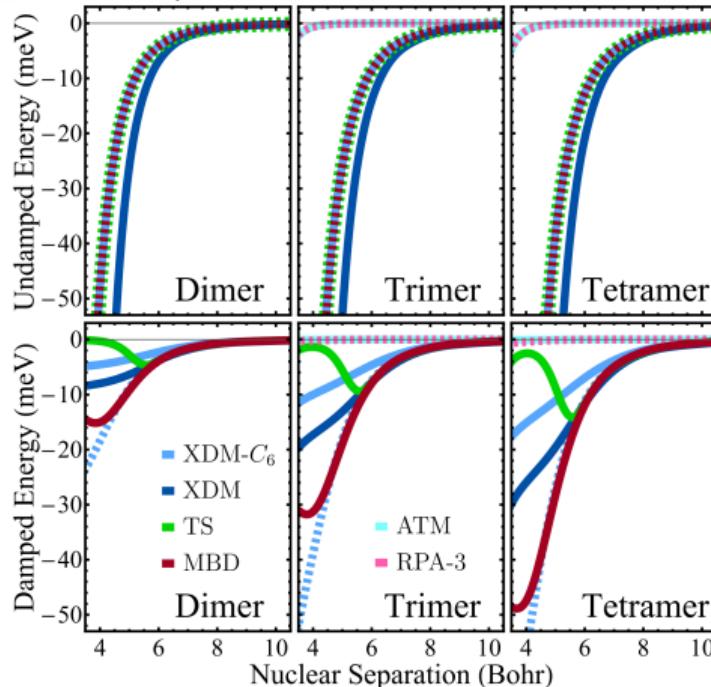
TETRAMER



MULTI-OSCILLATOR WAVEFUNCTIONS



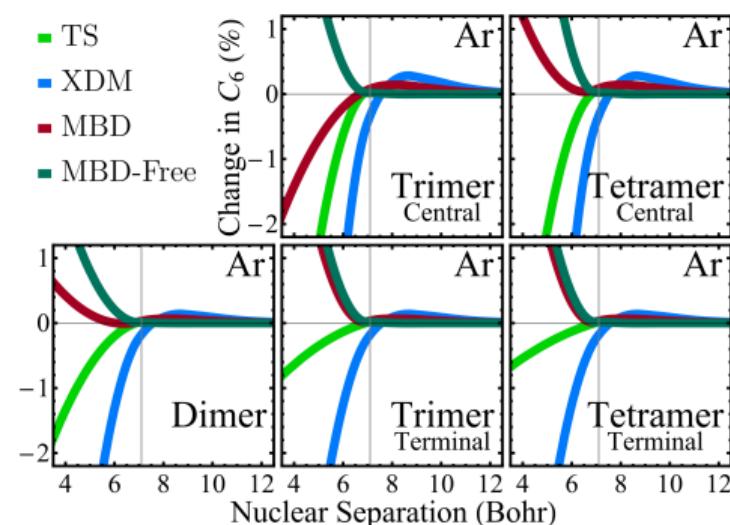
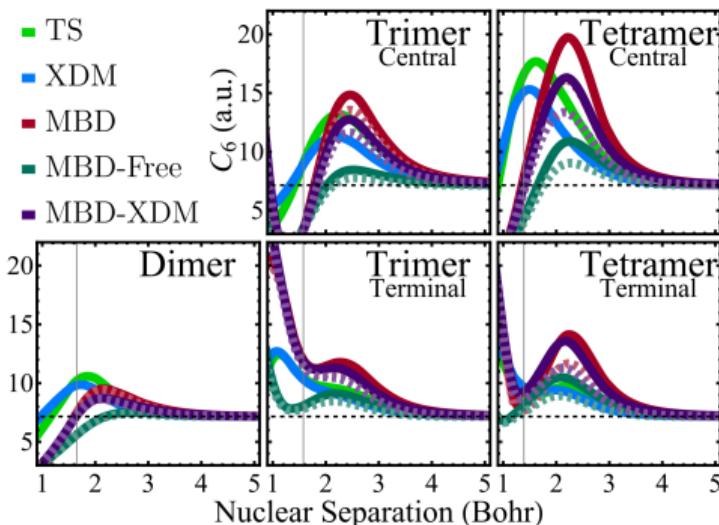
UNDAMPED/DAMPED ENERGY COMPARISON



- MBD seems to only be a C_6 -only method
- The 3-body dispersion energy contributions (ATM/RPA) are negligible
- C_6 -only corrections compensate by underdamping

OSCILLATOR CHAINS VS. ARGON CHAINS

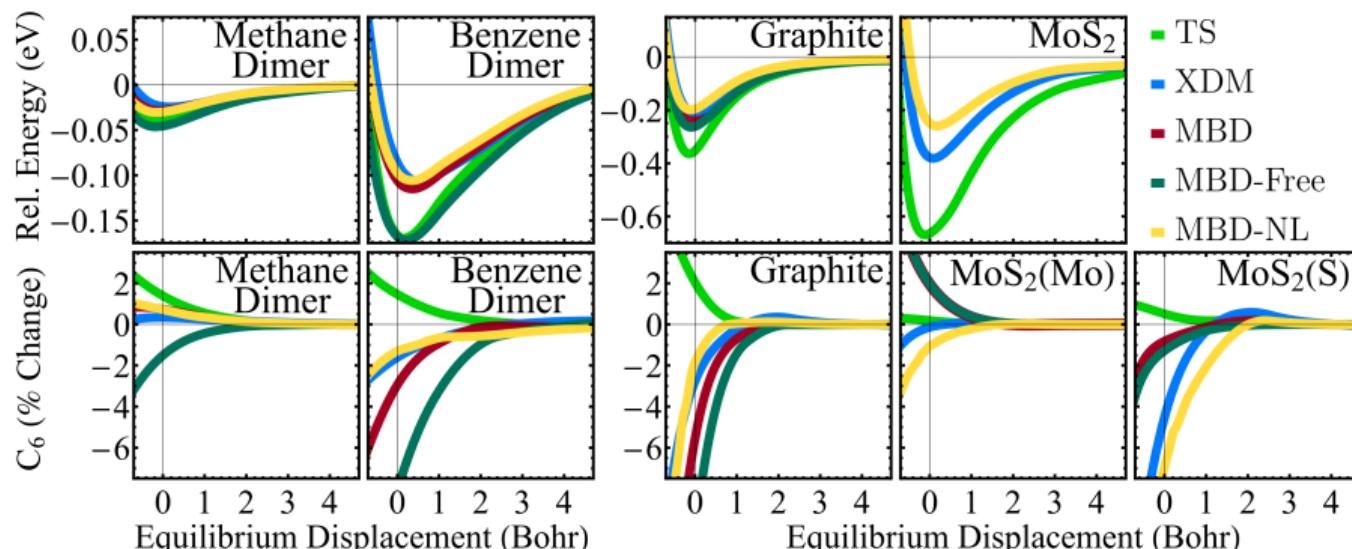
We compare to Ar chains as this model system will be bound by dispersion.
Computed in FHI-aims using tight basis settings and the PBE functional.



- All methods capture similar C_6 changes for oscillator chains, but less so in the Ar chains
- MBD is very sensitive to starting conditions, and has “polarization catastrophe” issues

CONNECTION WITH MOLECULAR DIMERS AND LAYERED MATERIALS

Computed in FHI-aims using the PBE functional and the lightdense basis.
For the layered materials, $12 \times 4 \times 4$ k -point meshes were used.



- MBD and MBD-Free fail for MoS_2
- XDM and MBD-NL are in general agreement
- TS is no longer showing the same responsiveness as in the model systems

BENCHMARK RESULTS

XDM and MBD-NL performed best on the benchmark sets.
 However, we see that XDM consistently underestimates C_6 for molecules.

Benchmarks computed in FHI-aims using PBE and the lightdense basis

Benchmark		TS	MBD	MBD-NL	XDM
S66×8	(kcal/mol)	0.60	0.44	0.43	0.45
LM11	(meV/Å ²)	12.5	—	5.0	3.7
LM26	(meV/Å ²)	13.1	—	4.6	4.9
MolC6	(MAPE %)	12.7	13.1	7.3	20.1
MolC6	(MPE %)	2.5	-3.2	-2.2	-18.2

Table comparing different post-SCF dispersion corrections (Completed)

Disp.	Damping	C_6	$> C_6$	Empiricism	Elec.	Atom.
TS:	WY	✓	✗	α, C_6, R_{vdw}	✗	✗
XDM:	BJ	✓	✓	α	$d_{X\sigma}$	C_9
MBD:	rsSCS	✓	✗	TS@SCS	SCS	\hat{H}_{CFDM}
MBD-NL:	rs	✓	✗	VV10	VV10	\hat{H}_{CFDM}
MBD-Free:	rsSCS	✓	✗	Free@SCS	SCS	\hat{H}_{CFDM}
MBD-XDM:	rsSCS	✓	✗	$d_{X\sigma}+SCS$	$d_{X\sigma}+SCS$	\hat{H}_{CFDM}

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XDM: The Exchange-Hole Dipole Moment Model

Inclusion of Dynamical Correlation: XCDM

A One-Parameter Damping Function: Z-Damping

Molecular and Solid-State Benchmarking

Conclusions

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 divergence at small interatomic separations, R_{ij} . The XDM model calculates the dispersion coefficients, C_n , using exchange-hole dipole moments,

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

which can be 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, ρ_σ , to compute the multipole moment integrals,

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

These are then combined with atom-in-molecule polarizabilities, α_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



SHORT-RANGE DYNAMICAL CORRELATION MODELS

Canonically, the exchange hole, $h_{X\sigma}$, used in XDM is 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

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

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:

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

The first scalar moment of the correlation hole,

$$d_C(\mathbf{r}) \approx \int h_C(\mathbf{r}, s) s d\mathbf{s},$$

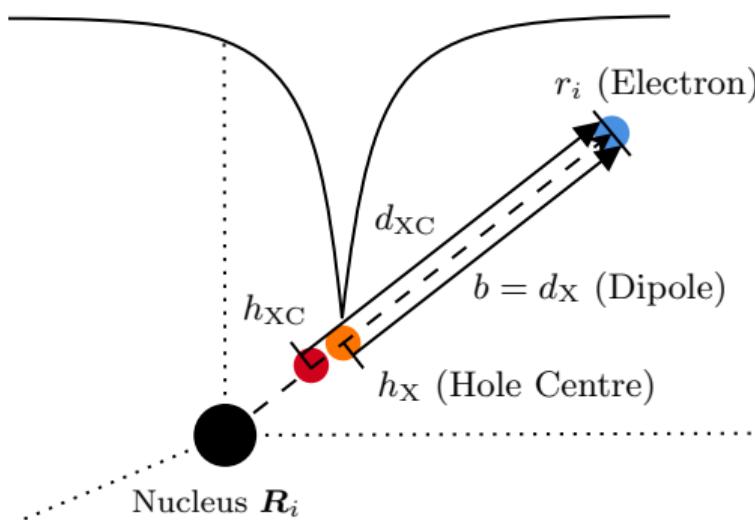
should provide a measure of the average distance between the reference electron and hole centre and will be used to approximate the correlation-hole dipole moment. The same- and opposite-spin correlation-hole dipole moment contributions are then

$$d_{C\sigma\sigma}(\mathbf{r}) = \left[\frac{g_{\sigma\sigma} z_{\sigma\sigma}^7}{2 + z_{\sigma\sigma}} D_\sigma(\mathbf{r}) \right], \quad d_{C\sigma\sigma'}(\mathbf{r}) = \left[\frac{g_{\sigma\sigma'} z_{\sigma\sigma'}^5}{1 + z_{\sigma\sigma'}} \rho_{\sigma'}(\mathbf{r}) \right].$$

The sech-type normalization function was ultimately chosen, resulting in $g_{\sigma\sigma} = 0.01243$ and $g_{\sigma\sigma'} = 0.5360$. The σ -spin exchange-correlation dipole moment is then given by

$$\begin{aligned} d_{XC\sigma}(\mathbf{r}) &= d_{X\sigma}(\mathbf{r}) + d_{C\sigma\sigma}(\mathbf{r}) + d_{C\sigma\sigma'}(\mathbf{r}) \\ &\approx b_\sigma + \left[\frac{g_{\sigma\sigma} z_{\sigma\sigma}^7}{2 + z_{\sigma\sigma}} D_\sigma \right] + \left[\frac{g_{\sigma\sigma'} z_{\sigma\sigma'}^5}{1 + z_{\sigma\sigma'}} \rho_{\sigma'} \right]. \end{aligned}$$

CORRELATION CONTRIBUTION TO THE BR EXCHANGE HOLE

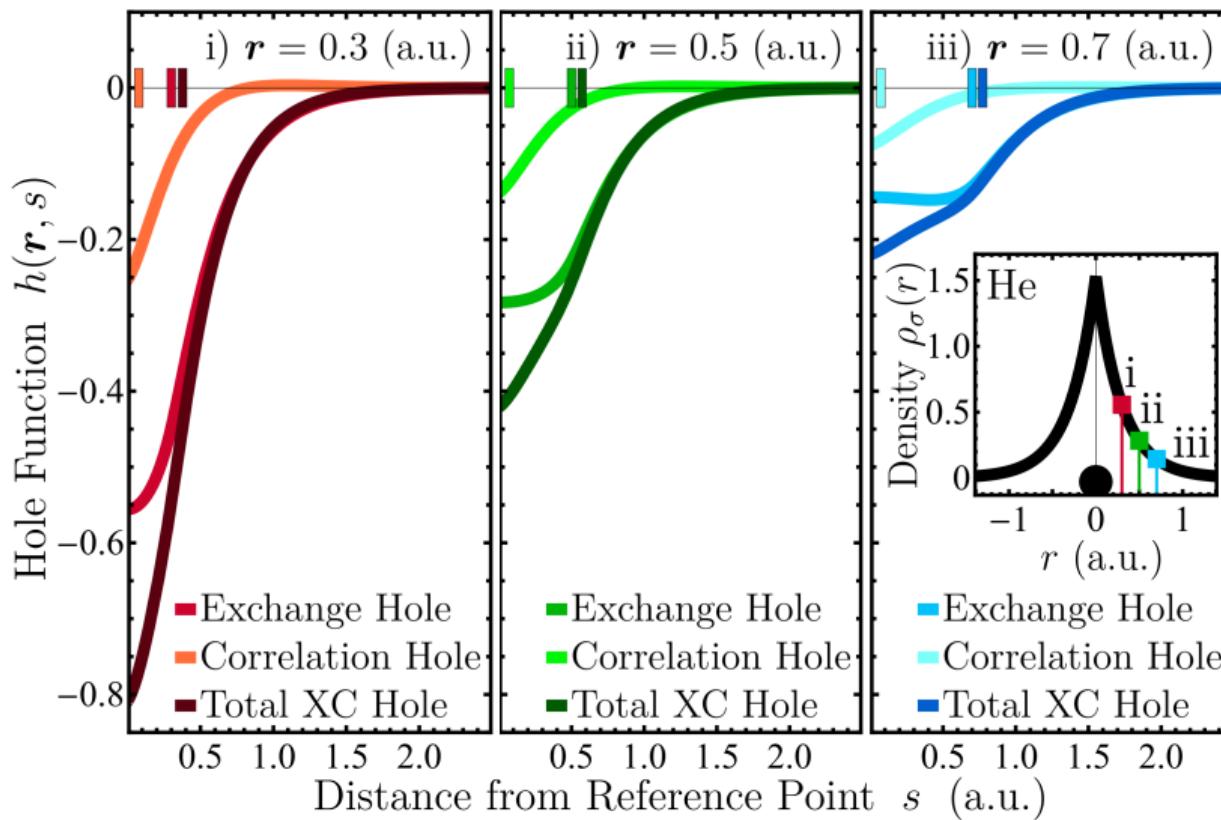


IMPROVEMENTS IN MOLECULAR C_6 COEFFICIENTS

Computed using FHI-aims with tight basis

MOLC6 Functional	XDM		XCDM	
	MAPE	MPE	MAPE	MPE
B86bPBE	18.4	-16.4	8.5	2.7
B86bPBE0	19.6	-18.1	8.6	0.6
B86bPBE50	17.0	-14.5	9.0	-1.2
PBE	18.1	-16.1	8.4	3.3
PBE0	19.4	-17.9	8.5	1.1
PBE50	16.6	-14.0	8.9	-0.9

PLOTS OF THE EXCHANGE-CORRELATION HOLE

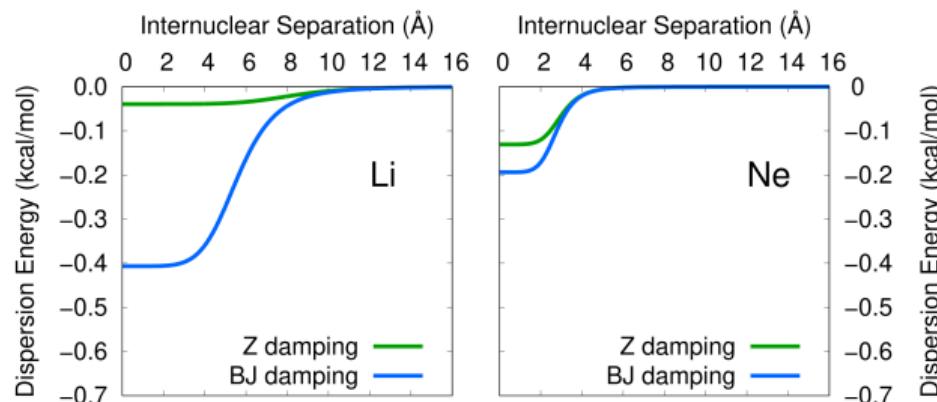


Z-DAMPING

The BJ-damping function, defined in terms of the “critical” interatomic distance at which successive dispersion energy terms become equal, and Z-damping, defined in terms of the atomic numbers, are given by

$$f_n^{\text{BJ}}(R_{ij}) = \frac{R_{ij}^n}{R_{ij}^n + (a_1 R_{c,ij} + a_2)^n}, \quad f_n^Z(R_{ij}) = \frac{R_{ij}^n}{R_{ij}^n + z_{\text{damp}} \frac{C_{n,ij}}{Z_i + Z_j}}.$$

The a_1 , a_2 , and z_{damp} parameters are optimised by minimizing the RMS percent error in binding energies for a set of 49 molecular dimers, KB49.



MOLECULAR AND SOLID-STATE BENCHMARKING

Basis Sets:

- light
- lightdense
- lightdenser
- intermediate
- tight
- tier2_aug2
- aug-cc-pvtz

Functionals:

- B86bPBE
- B86bPBE0
- B86bPBE-50
- PBE
- PBE0
- PBE-50
- HSE06
- LC- ω PBE
- LC- ω PBEh
- B3LYP
- BHLYP

Benchmarks:

C_6 Benchmark and Fit Set:

- MolC6 – Molecular C_6 Coefficients
- KB49 – Intermolecular Complexes

Molecular Benchmarks:

- GMTKN55 – General, Main Group Thermochemistry, Kinetics and Noncovalent Interactions

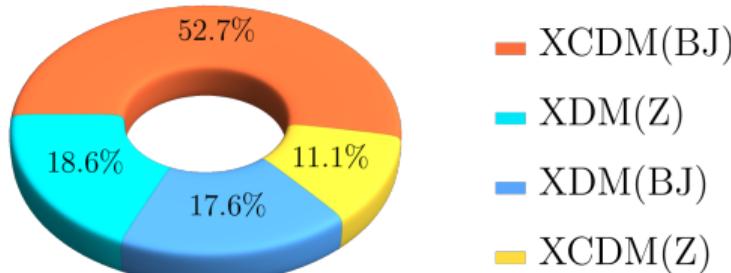
Solid-State Benchmarks:

- X23 – Molecular Crystals
- HalCrys4 – Halogen Crystals
- Ice13-Abs – Ice Crystal Phases (Absolute)
- Ice13-Rel – Ice Crystal Phases (Relative)
- LM26/11 – Layered Materials

XCDM and Z-damping are implemented in FHI-aims and PostG.

GMTKN55 KEY TAKEAWAYS

1. XCDM(BJ) has exceptional accuracy for molecular systems



Share of GMTKN55 where each dispersion method minimized MAD

2. Z-damping fixes overbinding in alkali metal crystals

Alk8 MAEs:

$$\begin{array}{ccc} \text{XDM(BJ)} & \rightarrow & \text{XDM(Z)} \\ 13.5 \text{ kcal/mol} & & 3.2 \text{ kcal/mol} \end{array}$$

$$\begin{array}{ccc} \text{XCDM(BJ)} & \rightarrow & \text{XCDM(Z)} \\ 9.9 \text{ kcal/mol} & & 3.0 \text{ kcal/mol} \end{array}$$

3. XDM methods perform very strongly compared to other dispersion corrections

GMTKN55 weighted MADs (kcal/mol)

Functional	DC	WTMAD-2	WTMAD-4
PBE0	D3(BJ)	6.60	5.87
PBE0	TS	6.53	6.43
PBE0	MBDrSCS	6.45	6.12
PBE0	MBD-NL	6.53	6.16
PBE0	XDM(BJ)	6.55	6.06
PBE0	XDM(Z)	6.96	6.12
PBE0	XCDM(BJ)	6.23	5.79
PBE0	XCDM(Z)	6.88	6.06
B86bPBE0	XDM(BJ)	5.78	5.34
B86bPBE0	XDM(Z)	6.43	5.73
B86bPBE0	XCDM(BJ)	5.59	5.23
B86bPBE0	XCDM(Z)	6.29	5.60
LC- ω PBE	XDM(BJ)	5.48	5.98
LC- ω PBE	XDM(Z)	5.51	5.92
LC- ω PBE	XCDM(BJ)	5.67	6.20
LC- ω PBE	XCDM(Z)	5.44	5.85

4. LC- ω PBE-XCDM(Z) has best-in-class performance for GGA-based RS-hybrids

SOLID STATE RESULTS

Basis-set corrected MAEs, in kcal/mol

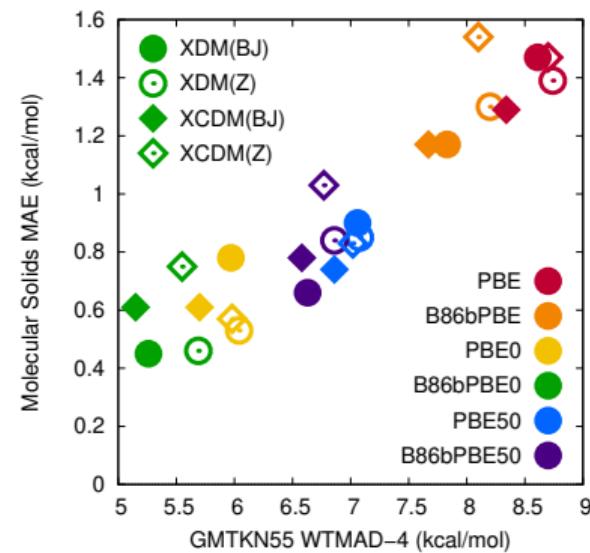
X23 Functional	XDM		XCDM	
	BJ	Z	BJ	Z
PBE	1.13	0.92	0.63	0.98
B86bPBE	0.70	0.81	0.63	1.20
PBE0	1.00	0.66	0.53	0.74
B86bPBE0	0.48	0.61	0.65	1.19
PBE50	0.87	0.75	0.60	0.79
B86bPBE50	0.51	0.73	0.73	1.24

tight MAEs, in kcal/mol/cell

LM11 Functional	XDM		XCDM	
	BJ	Z	BJ	Z
B86bPBE	1.5	1.4	3.6	3.3
PBE	1.3	1.0	3.3	2.5

OVERALL OBSERVATIONS

- XCDM(BJ) has improved performance for molecular systems and X23, but struggles with layered materials
- Z-damping resolves the issues with alkali metal crystals, consistent across the solid state, and great for layered materials



PhD Contributions
oo

Introduction
oooooo

Oscillators Project
ooooooo

XCDM Project
oooooooooooo

Conclusions
ooo

PhD Contributions

Introduction

Oscillators Project

XCDM Project

Conclusions

CONCLUDING REMARKS

1. XDM has demonstrated its ability to capture the physics of London dispersion, to deliver best-in-class energies across many diverse systems, and has a stable implementation that avoids crashes that affect some competing methods
2. New, physics-guided implementations of XDM were introduced, incorporating the missing contributions from dynamical correlation (XCDM), and reducing empiricism with Z-damping
3. These developments were rigorously tested and benchmarked, and implemented in open-source software: FHI-aims and PostG

ACKNOWLEDGEMENTS



The Johnson Group:

Current:

- Prof. Erin Johnson
- Em. Prof. Axel Becke
- Adrian Rumson
- Cameron Nickerson
- Grace Sparrow
- Laura Rizzo
- Sam Petrov
- Lindsay Hurshman
- Mike Cotnam
- Mohammad Rafiee Diznab

Recent Alumni:

- Adebayo Adeleke
- Alex Mayo
- Alastair Price
- Sarah Clarke
- Nick Roberts
- Joseph Weatherby
- Fouad Kaadou
- Xibo "Fred" Feng
- Tilas Kabengele
- Sam Dudra

Funding and Resources:

- Killam Trusts
- Dalhousie University
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- Digital Research Alliance of Canada
- ACENET
- FHI-aims

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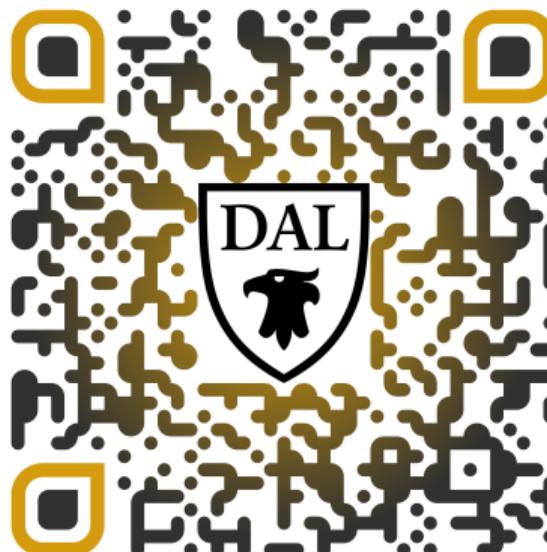
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QUESTIONS?

WANT MY SLIDES/THESIS?



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

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