

# **Putting a spin on time dependent electronic structure theory**

**Joshua Goings  
General Exam**

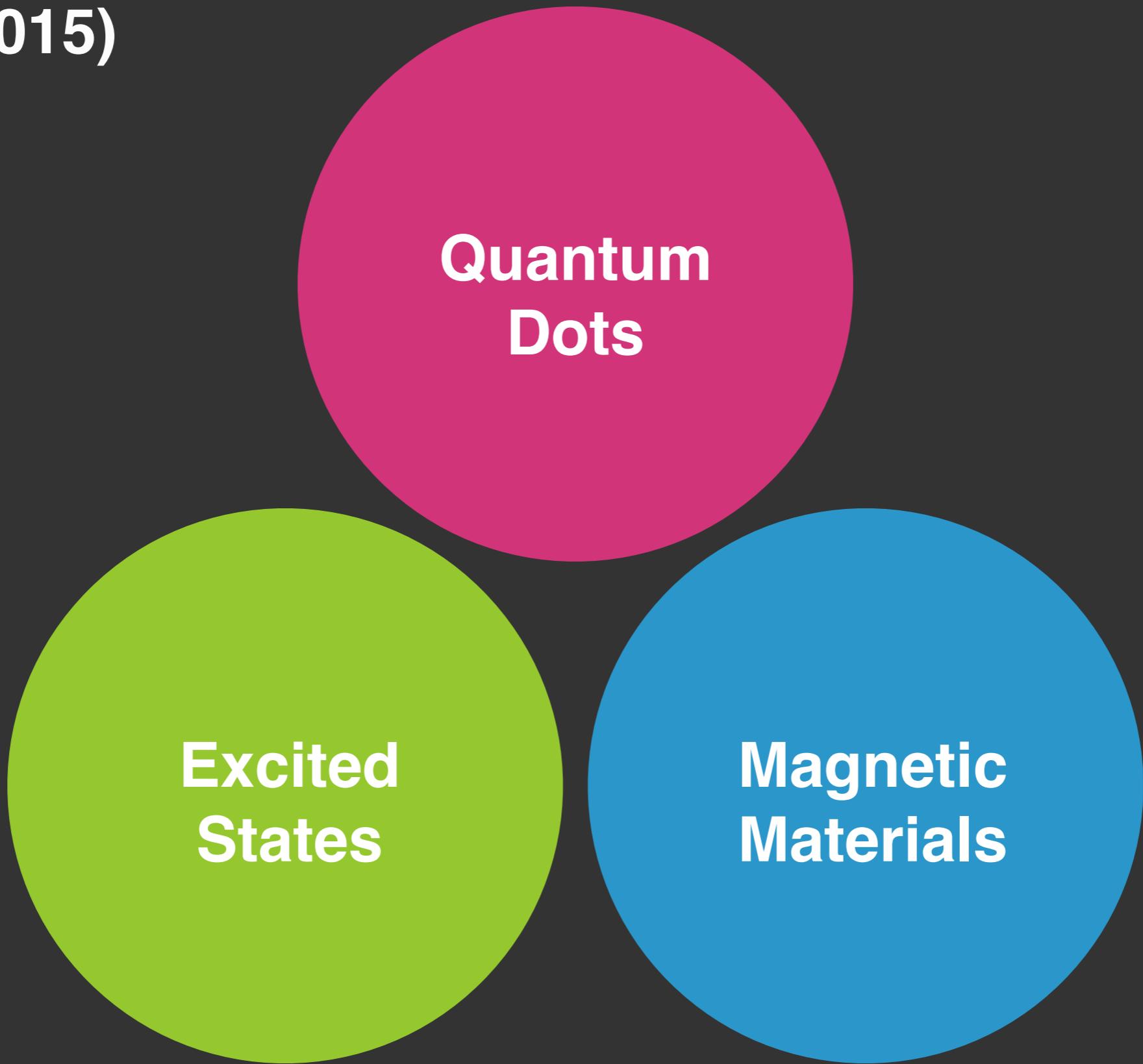
**Thursday, May 14, 10:00am CHB 339**

# **Thank you to General Exam Committee**

**Xiaosong Li (chair)**  
**Jim Pfaendtner (GSR)**  
**Matthew Bush**  
**David Masiello**  
**Stefan Stoll**

**How can we predict and understand  
the electronic and magnetic responses  
of molecules and nano-materials?**

# Research Directions (2014–2015)



# Research Directions (2014–2015)

Excited States

1. Goings, J. J., Caricato, M., Frisch, M. J., & Li, X. (2014). *JCP*, **141**(16), 164116.

Quantum Dots

2. Goings, J. J., Schimpf, A. M., May, J. W., Johns, R. W., Gamelin, D. R., & Li, X. (2014). *JPC C*, **118**(46), 26584.

Magnetic Materials

3. Ding, F., Goings, J. J., Frisch, M. J., & Li, X. (2014). *JCP*, **141**(21), 214111.
4. Goings, J. J., Ding, F., Frisch, M. J., & Li, X. (2015). *JCP*, **142**(15), 154109.

Other

5. Goings, J. J., Ohlsen, S. M., Blaisdell, K. M., & Schofield, D. P. (2014). *JPC A*, **118**(35), 7411.
6. Goings, J. J., Ding, F., & Li, X. (2014). *Proceedings of MEST 2012: Electronic Structure Methods with Applications to Experimental Chemistry*, **68**, 77.

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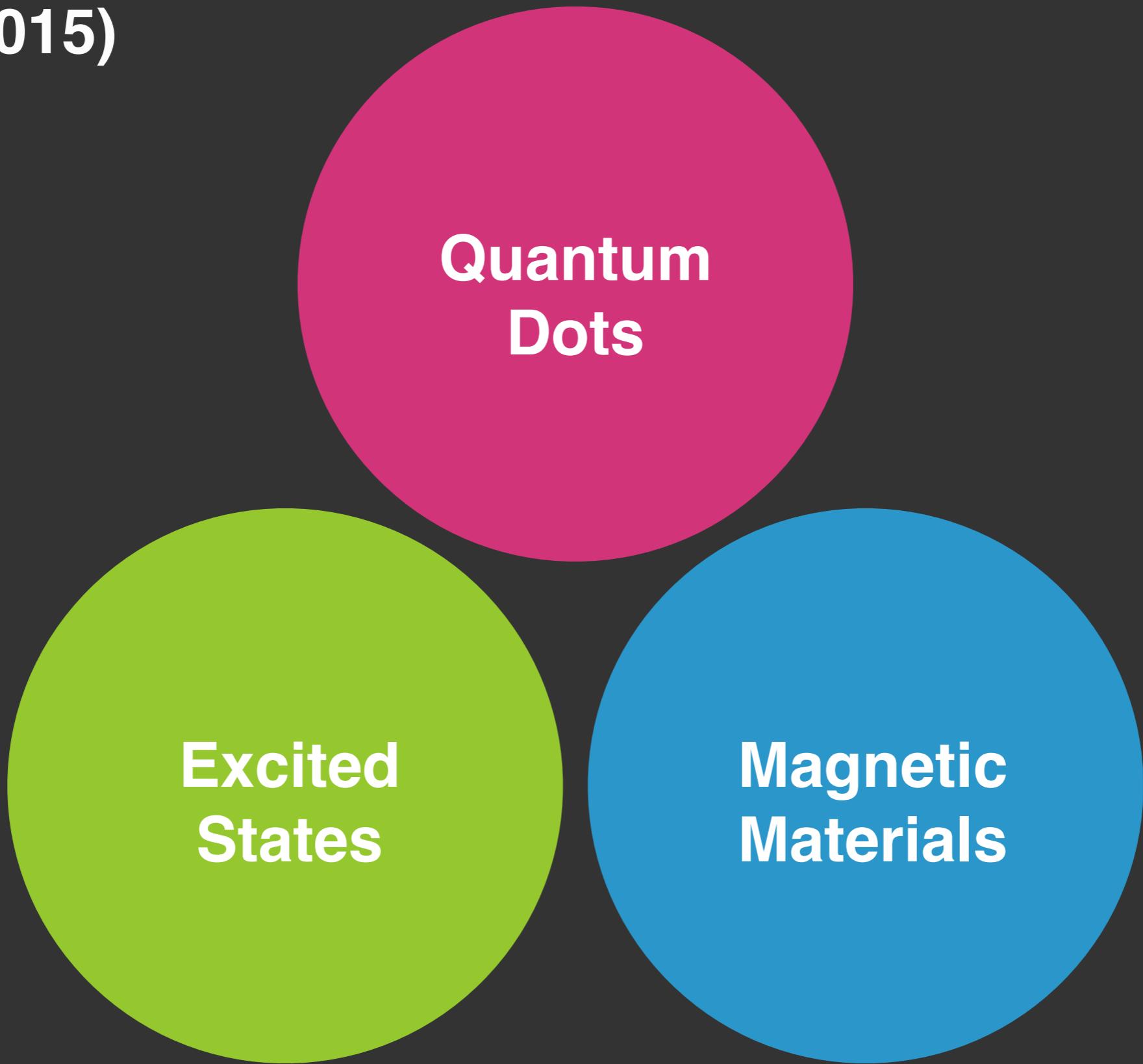
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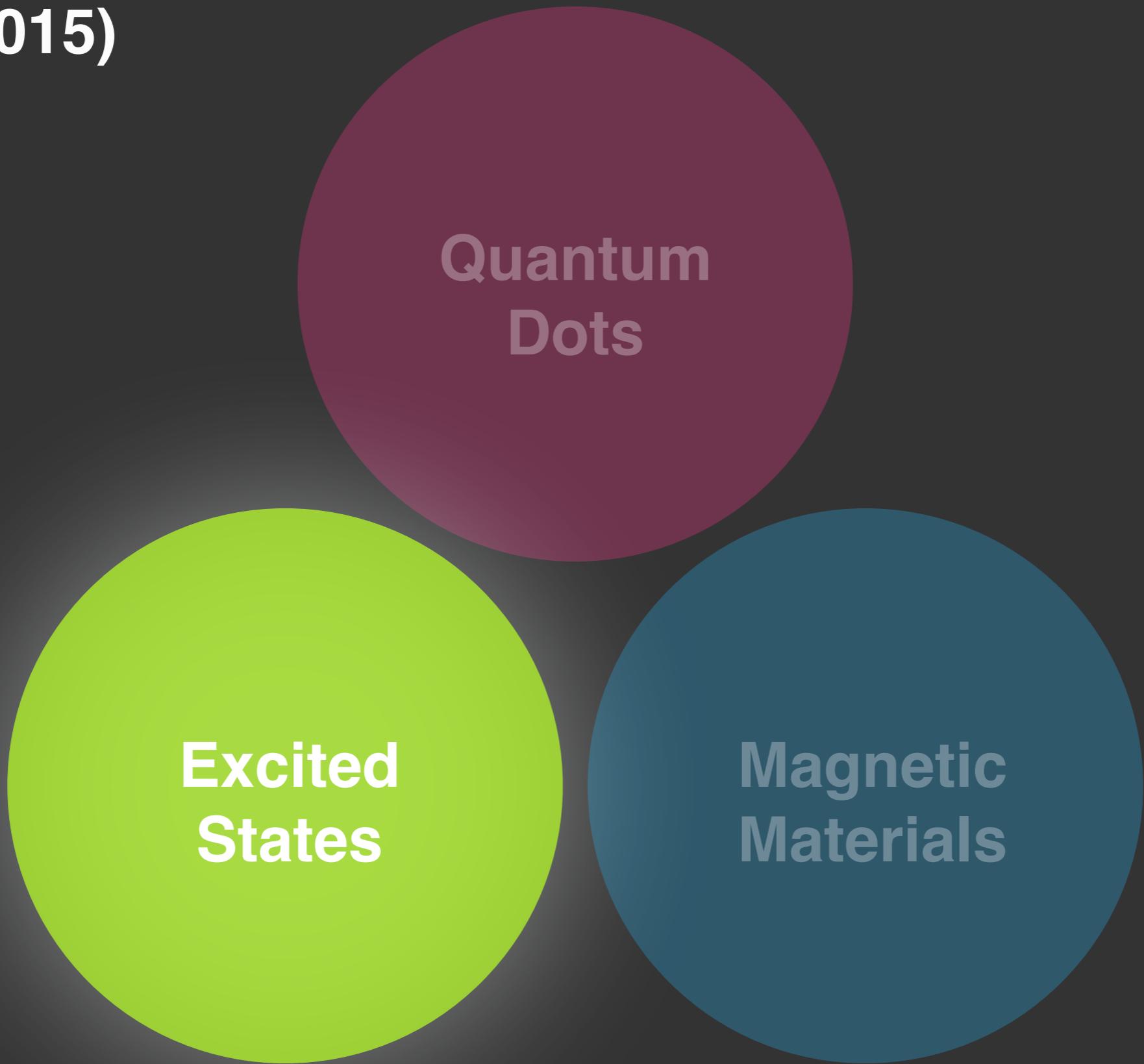
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# Research Directions (2014–2015)



# Research Directions (2014–2015)



## Excited States

# Balancing Cost + Accuracy of Electronic Excited State Methods

### LR-TDDFT

- $O(N^4)$
- Unpredictable
- No excited state exchange kernel
- Limited to single electron phenomena

### EOM-CCSD

- $O(N^6)$
- Systematically improvable
- Excited state electron correlation
- Multi-electron phenomena

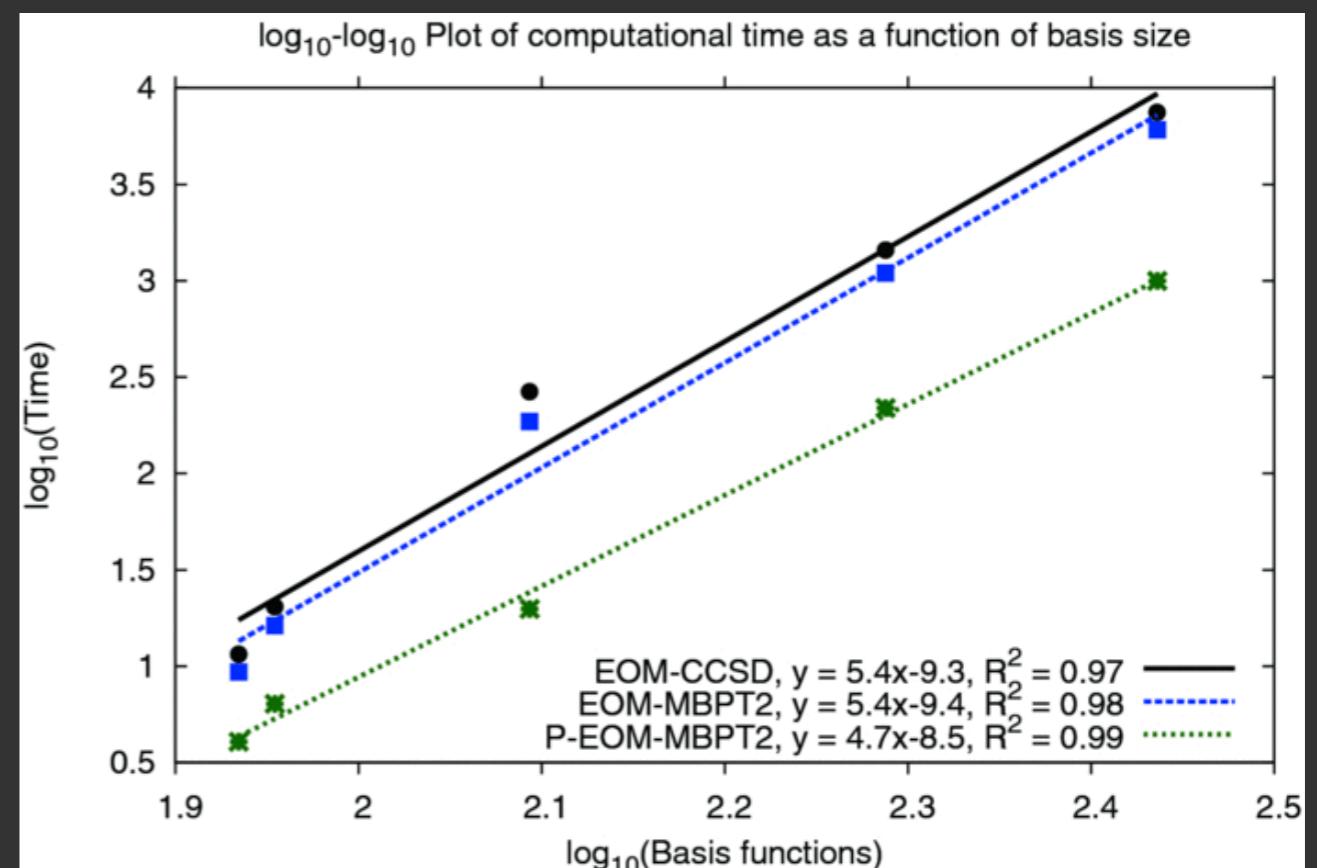
**Balance cost  
+ accuracy**

**(P)-EOM-  
MBPT2,  
CC2, etc.**

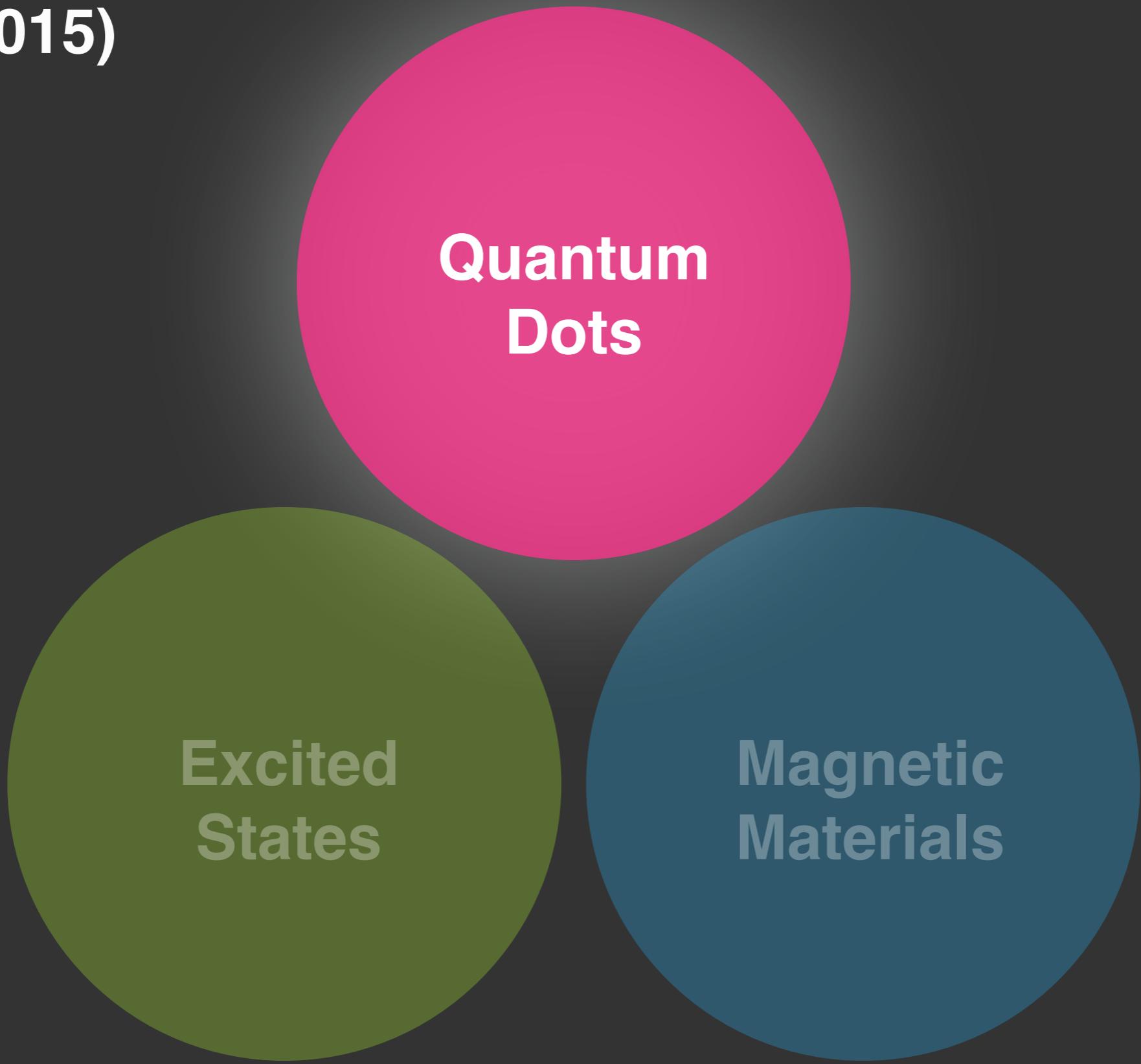
# Excited States

## Balancing Cost + Accuracy of Electronic Excited State Methods

- Applied perturbation theory to coupled cluster (CC) equations
- Reduced computational time of CC equations by an order of magnitude
- Accuracy generally outperforms density functional theory



# Research Directions (2014–2015)



# Quantum Dots

## Understanding Dopant Influence on Excitations in n-type Quantum Dots

$\text{Al}^{3+}:\text{ZnO}$

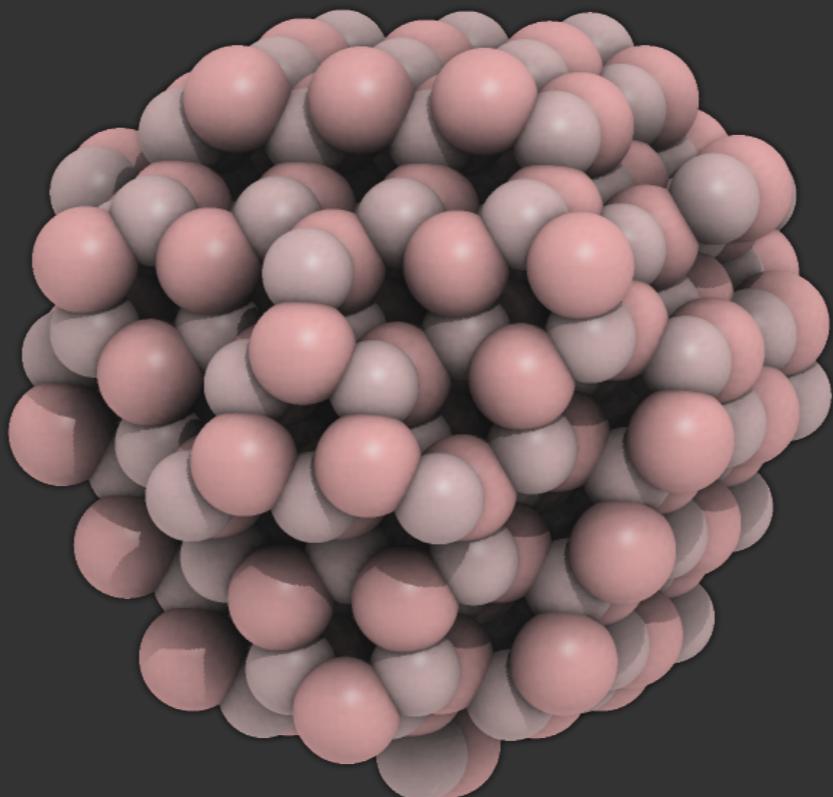
extra conduction  
band electron

tough to oxidize

$e^-:\text{ZnO}$

extra conduction  
band electron

easy to oxidize

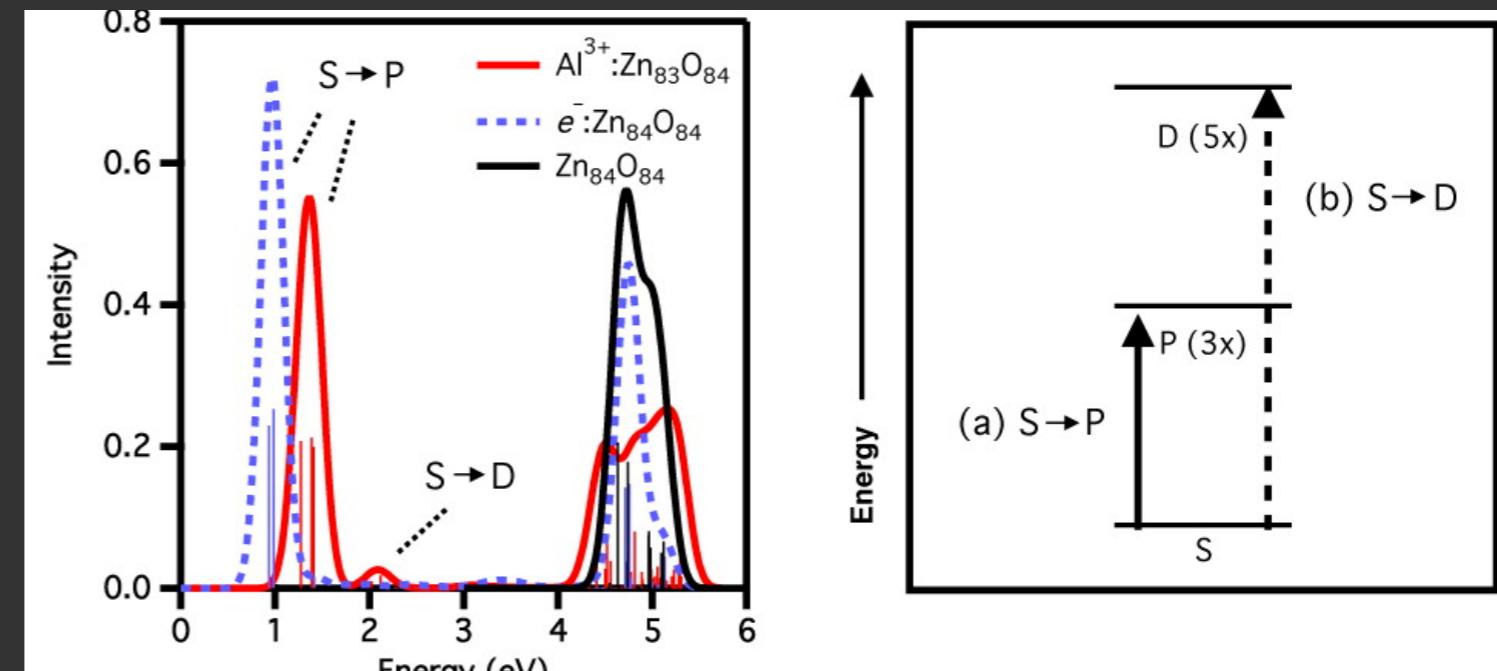


Goings, J. J., Schimpf, A. M., May, J. W., Johns, R. W., Gamelin, D. R., & Li, X. (2014). Theoretical Characterization of Conduction-Band Electrons in Photodoped and Aluminum-Doped Zinc Oxide (AZO) Quantum Dots. JPC C, 118(46), 26584-26590.

# Quantum Dots

## Understanding Dopant Influence on Excitations in n-type Quantum Dots

- n-type ZnO QDs
- UV-Vis spectra from aluminum doped and photodoped QDs
- Rationalized theoretical/experimental results in terms of particle-in-a-sphere



Goings, J. J., Schimpf, A. M., May, J. W., Johns, R. W., Gamelin, D. R., & Li, X. (2014). Theoretical Characterization of Conduction-Band Electrons in Photodoped and Aluminum-Doped Zinc Oxide (AZO) Quantum Dots. JPC C, 118(46), 26584-26590.

# Quantum Dots

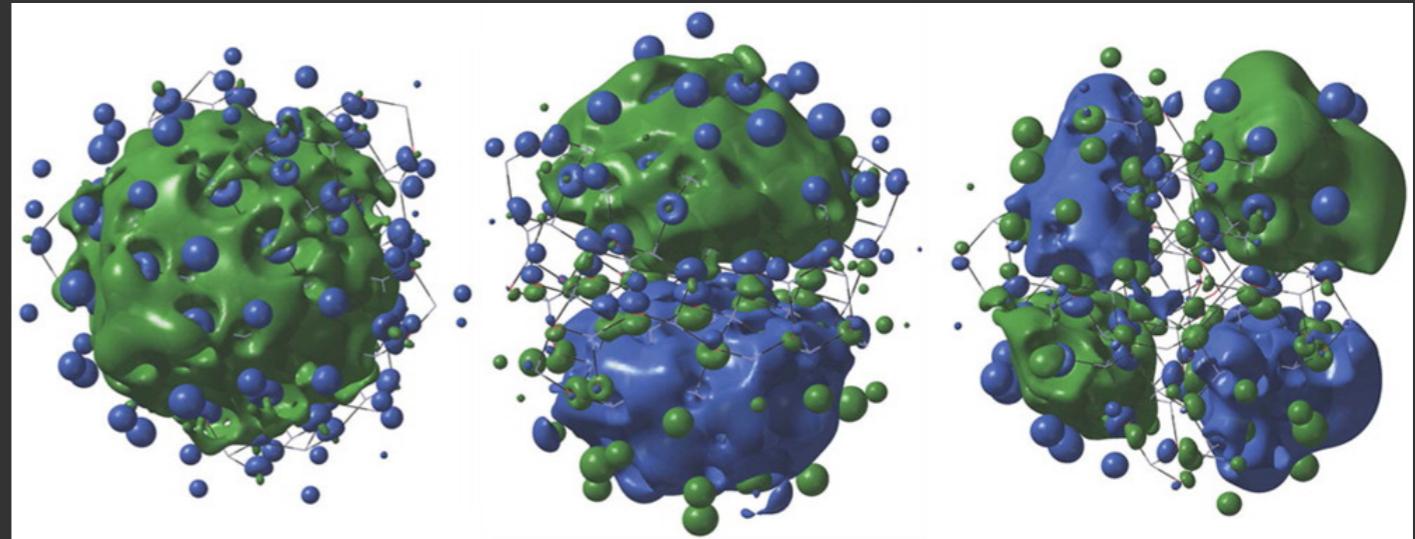
## Understanding Dopant Influence on Excitations in n-type Quantum Dots

- n-type ZnO QDs
- UV-Vis spectra from aluminum doped and photodoped QDs
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S

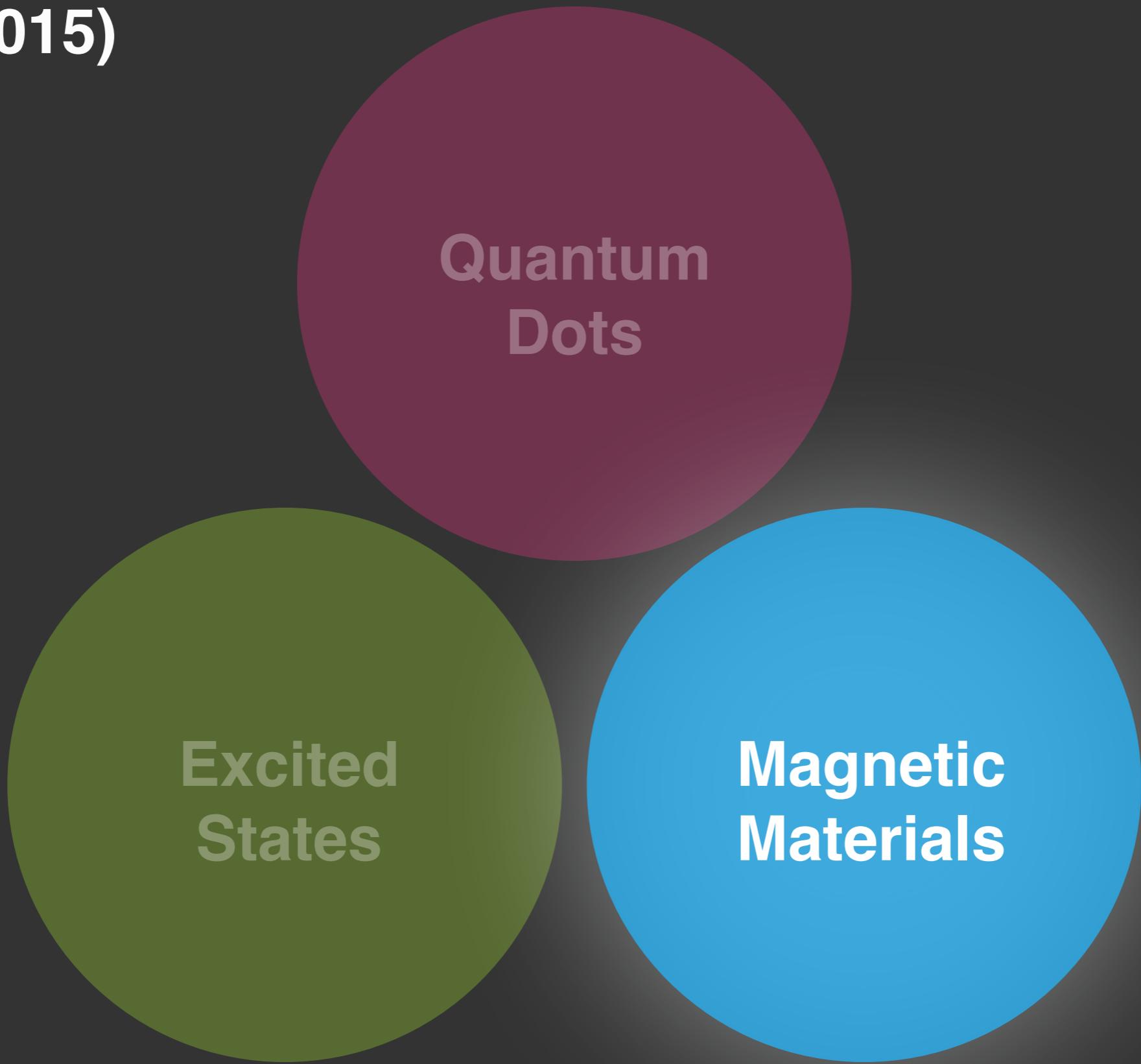
P

D



Goings, J. J., Schimpf, A. M., May, J. W., Johns, R. W., Gamelin, D. R., & Li, X. (2014). Theoretical Characterization of Conduction-Band Electrons in Photodoped and Aluminum-Doped Zinc Oxide (AZO) Quantum Dots. JPC C, 118(46), 26584-26590.

# Research Directions (2014–2015)

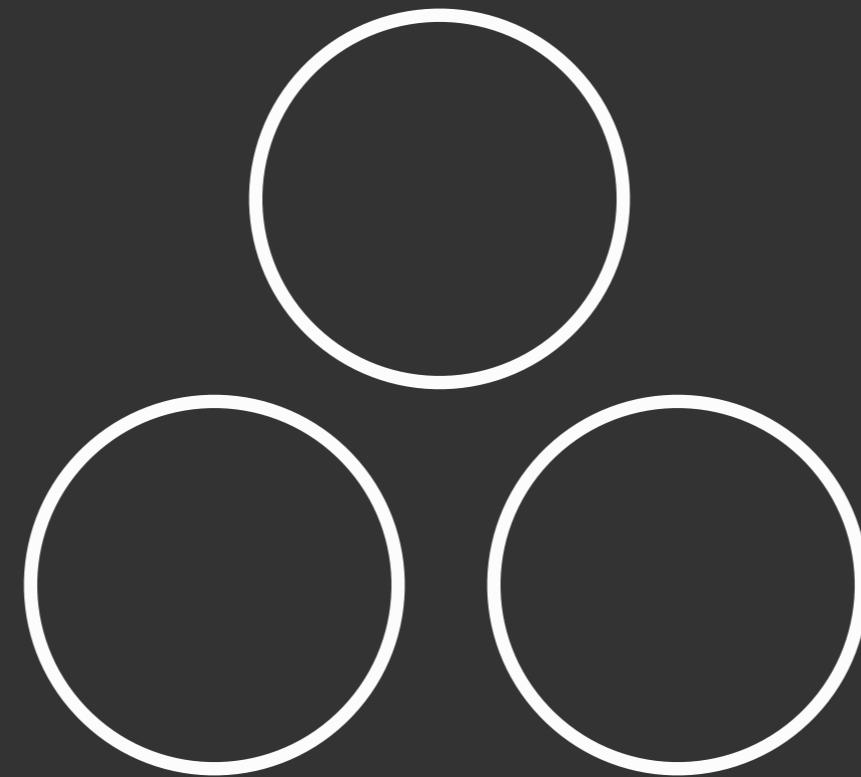


# Magnetic Materials

**Exploring spin-frustrated molecules  
with the generalized Hartree Fock (GHF) method**

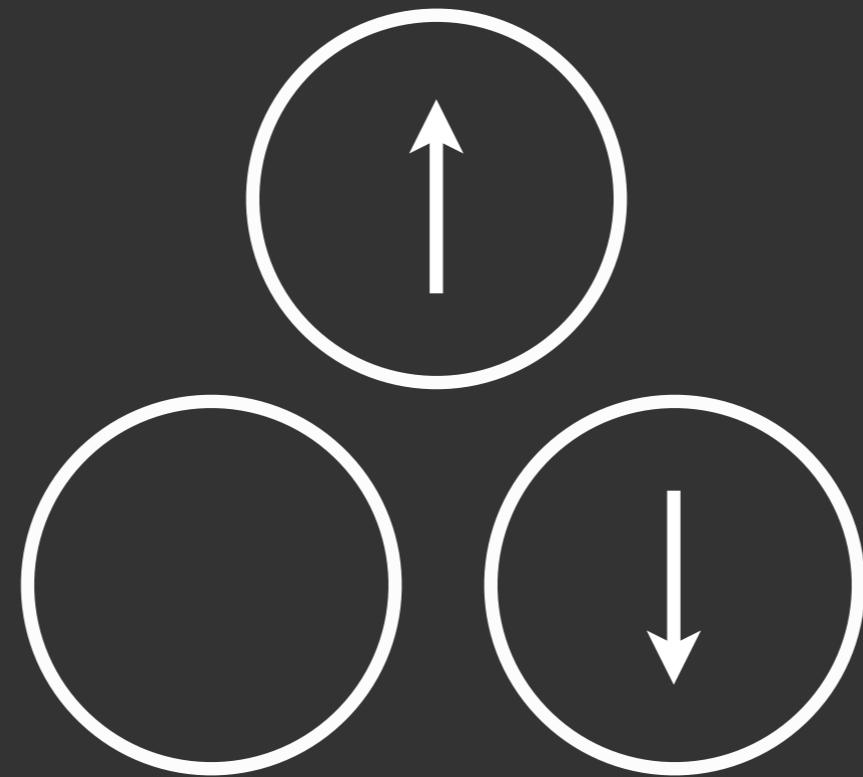
**Goings, J. J., Ding, F., Frisch, M. J., & Li, X. (2015). Stability of the complex generalized Hartree-Fock equations. The Journal of chemical physics, 142(15), 154109.**

# Magnetic Materials



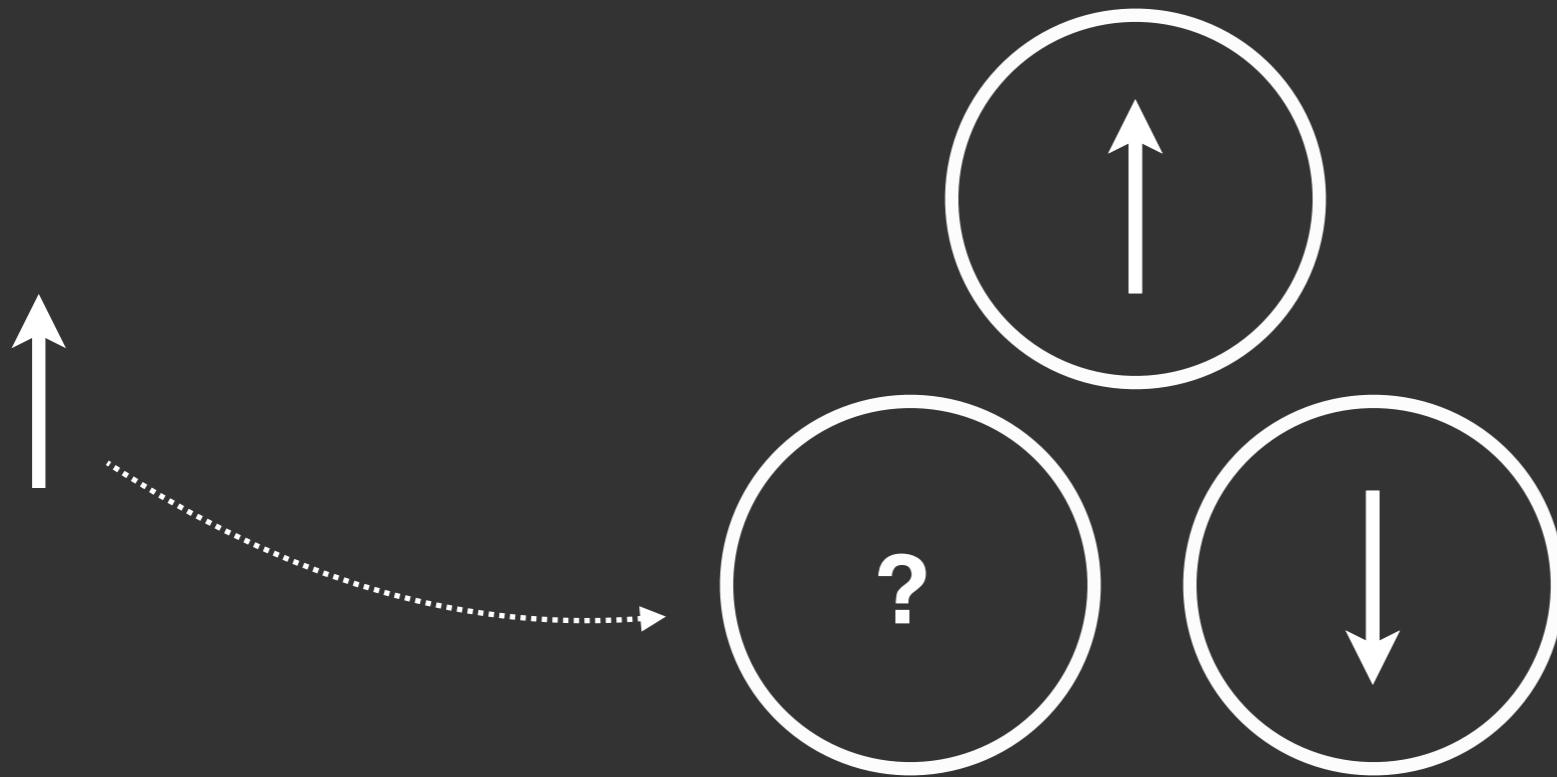
Take a three site lattice

# Magnetic Materials



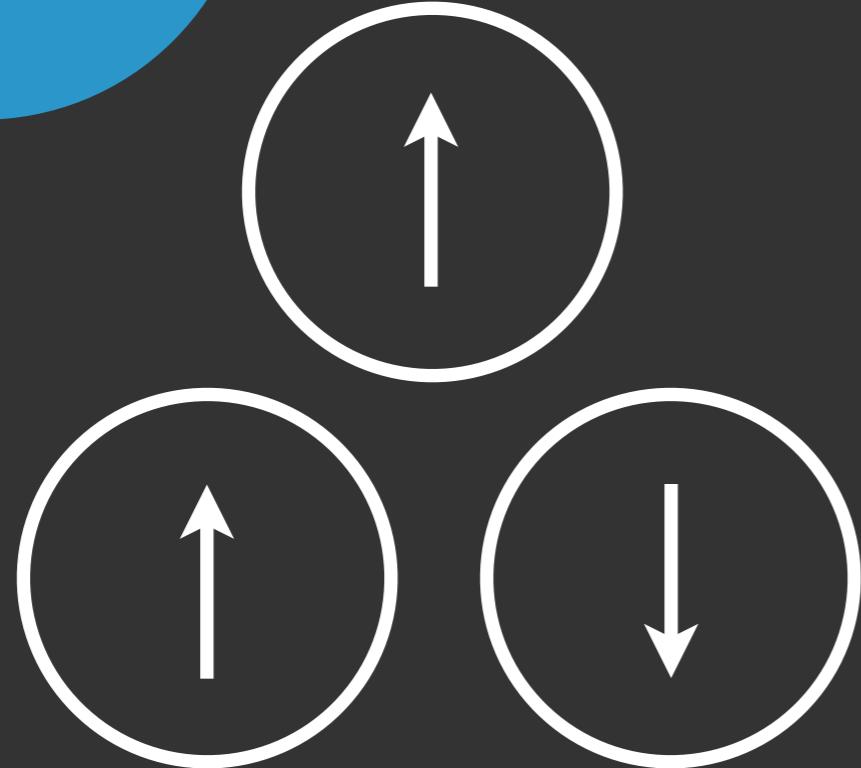
**Now add two electrons  
(assume antiferromagnetism is favored)**

# Magnetic Materials

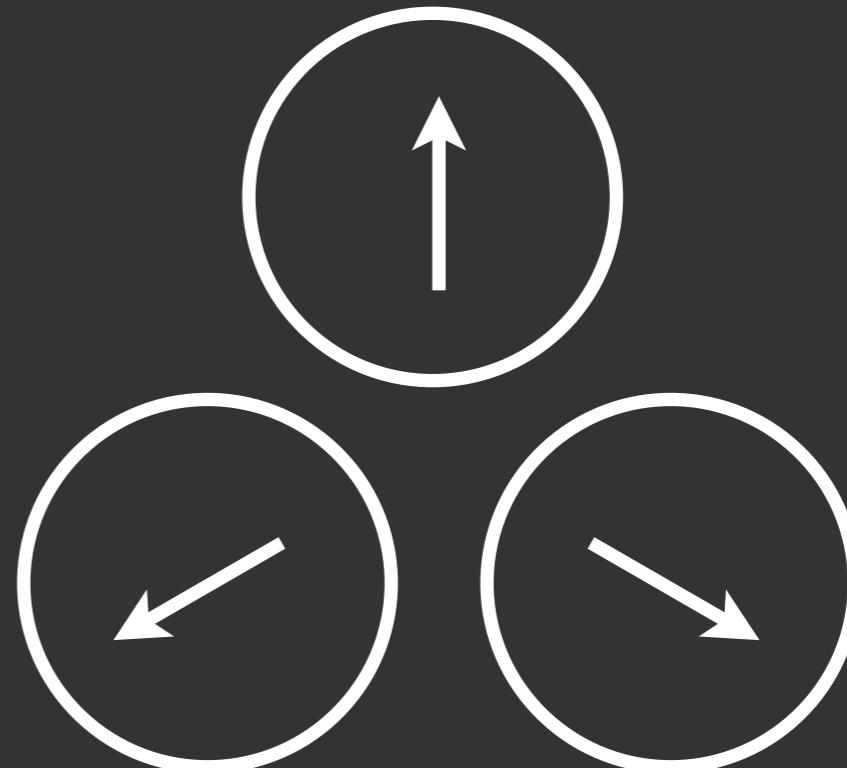


**Now add the third electron.  
No orientation simultaneously favors  
all anti-ferromagnetic interactions.**

# Magnetic Materials



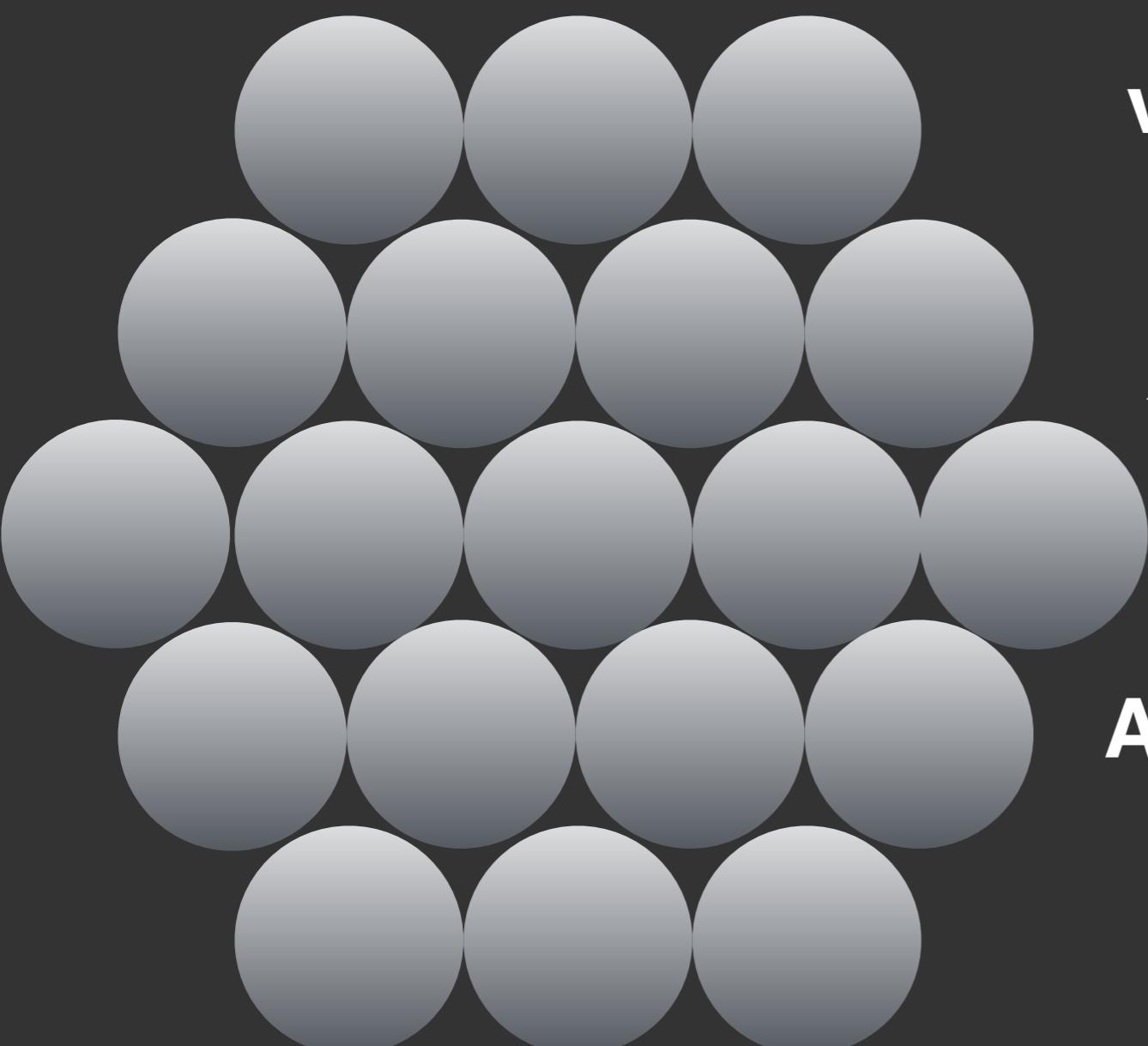
Collinear



Non-collinear

Conventional methods force you to pick a collinear configuration.  
Few methods can give you non-collinear state.

# Magnetic Materials

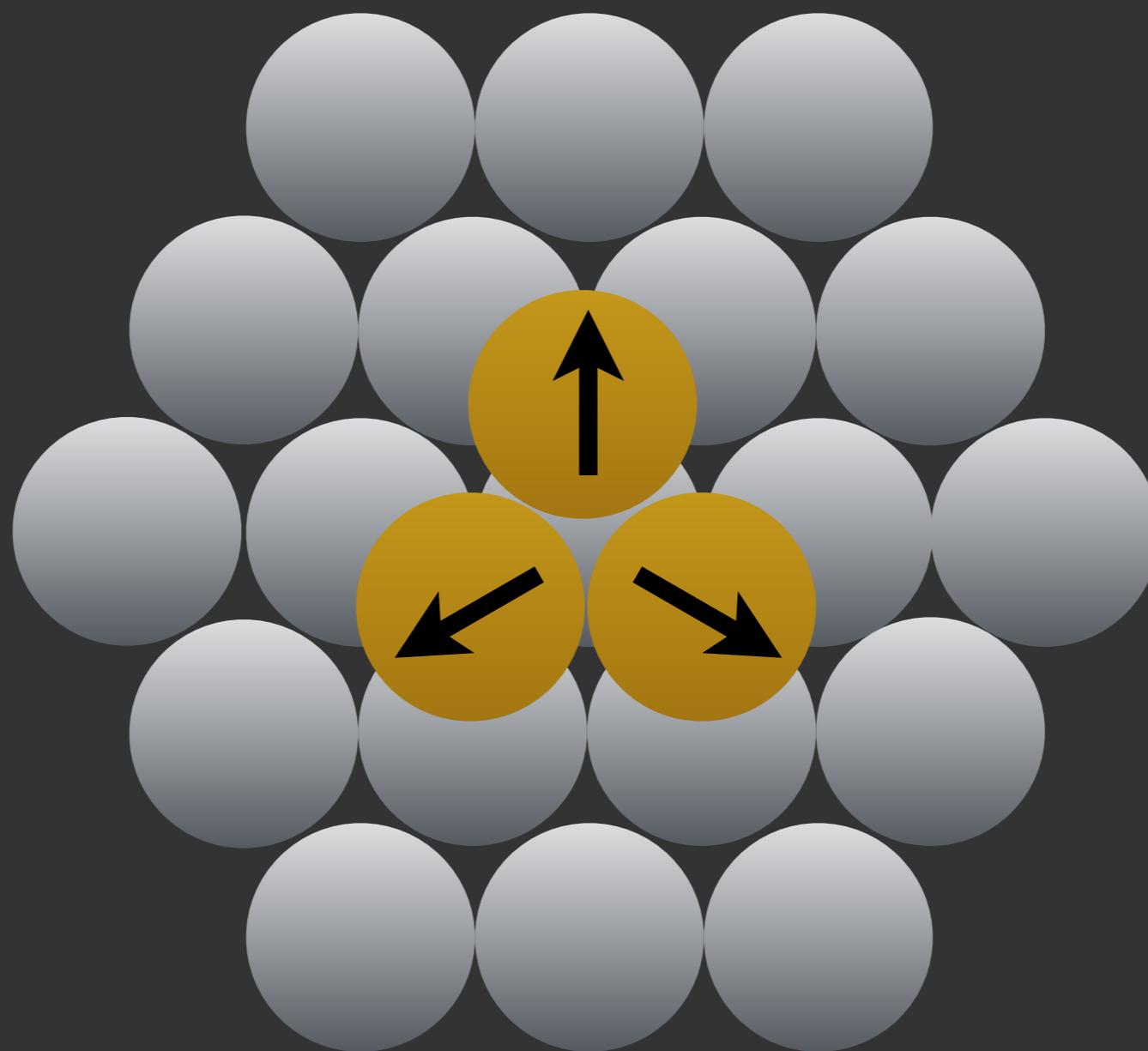


via STM

$\text{Cr}_3$

Ag fcc(111) surface

# Magnetic Materials



# Magnetic Materials

Can we describe this with Hartree Fock (HF)?

## Hartree-Fock (HF): minimize the energy of a single Slater Determinant

$$E \leq \frac{\langle \phi | \hat{H} | \phi \rangle}{\langle \phi | \phi \rangle}$$

The solution is **variational**; an upper bound to the exact energy.

This is an independent particle model (IPM). It is the quantitative basis of molecular orbital theory.

# Magnetic Materials

## Types of Hartree-Fock

	<b>Restricted (RHF)</b>	<b>Unrestricted (UHF)</b>	<b>General (GHF)</b>
<b>orbital</b>	spatial	$\phi(\mathbf{r})\alpha(\omega); \phi(\mathbf{r})\beta(\omega)$	$\phi(\mathbf{r})\alpha(\omega) + \phi(\mathbf{r})\beta(\omega)$
$\hat{S}^2$	yes	no	no
$\hat{S}_z$	yes	yes	no
<b>system</b>	closed shell	open shell	spin frustrated



Magnetic  
Materials

## Generalized Hartree Fock (GHF)

- GHF allows you to change spin smoothly

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- GHF allows you to change spin smoothly
- Lowest energy HF solution possible

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## Generalized Hartree Fock (GHF)

- GHF allows you to change spin smoothly
- Lowest energy HF solution possible
- Largely insensitive to guess multiplicity
- Only HF method to treat spin frustration

# Magnetic Materials

## Problem:

Just because you *can* get the lowest energy solution, doesn't mean you will.

## How to obtain GHF local minima?

unstable

stable

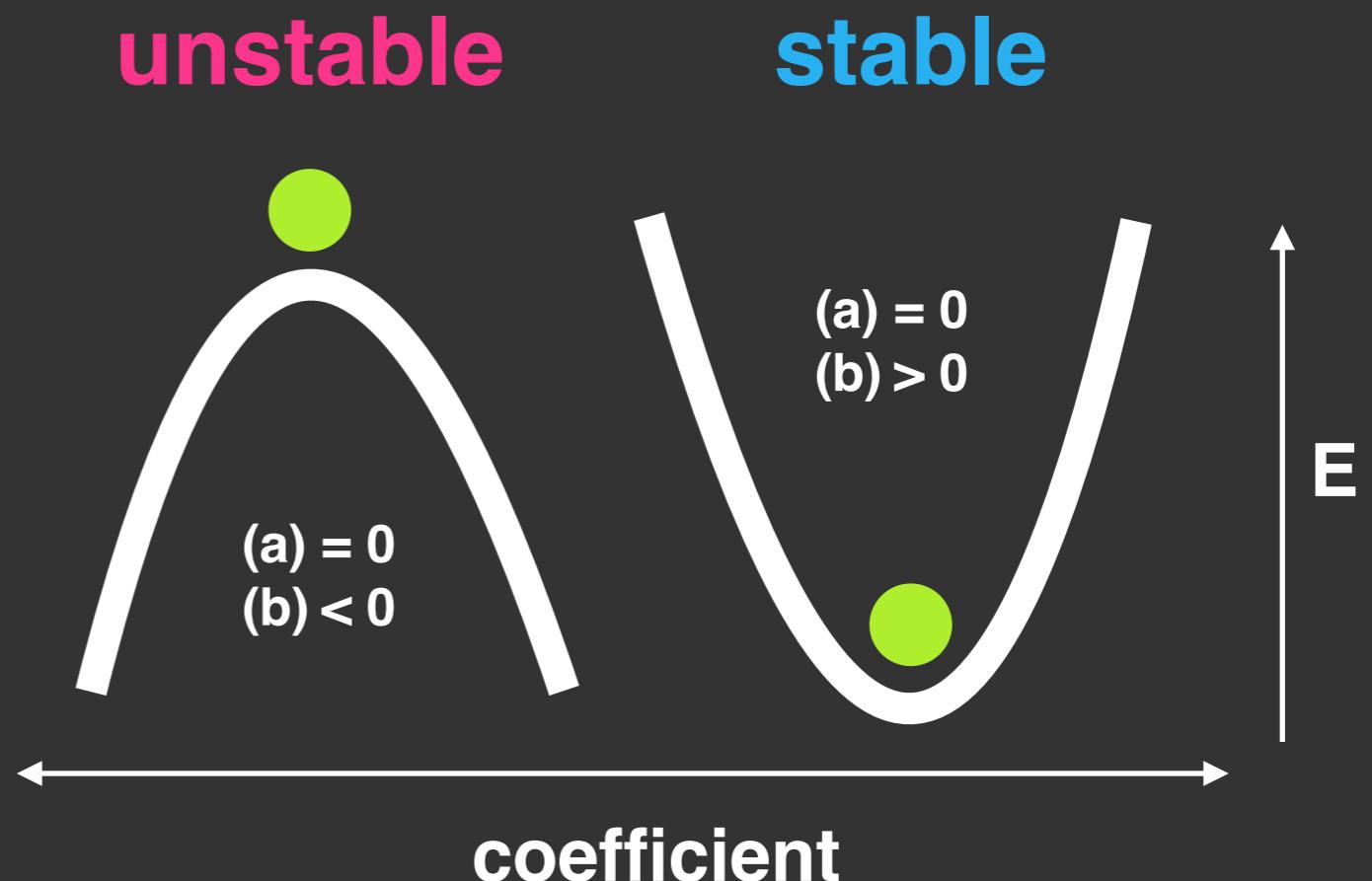


## How to obtain GHF local minima?

We want stable electronic solutions to the GHF model.

Local minima:

- (a) First variation equal to zero
- (b) Second variation greater than zero



# Magnetic Materials

Differentiate E with respect to wave function coefficients

$$\frac{\partial E}{\partial q_i^a} = \begin{pmatrix} \langle \phi_i^a | \hat{H} | 0 \rangle \\ \langle 0 | \hat{H} | \phi_i^a \rangle \end{pmatrix} = \begin{pmatrix} f_{ai} \\ f_{ia} \end{pmatrix}$$

This must equal zero, known as **Brillouin's theorem**.

(Trivially satisfied as long as HF converges to *something*)

## Second derivative of energy with respect to wave function coefficients

$$\frac{\partial^2 E}{\partial q_i^a \partial q_j^b} = \begin{pmatrix} \langle \phi_i^a | \hat{H} | \phi_j^b \rangle & \langle \phi_{ij}^{ab} | \hat{H} | 0 \rangle \\ \langle 0 | \hat{H} | \phi_{ij}^{ab} \rangle & \langle \phi_j^b | \hat{H} | \phi_i^a \rangle \end{pmatrix}$$

The Hessian, which must be **positive definite** if our solution is to be a minimum.

# Magnetic Materials

$$\text{Hessian} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$$

$$A_{ia,jb} = (\epsilon_a - \epsilon_i) \delta_{ia,jb} + \langle aj || ib \rangle, \quad B_{ia,jb} = \langle ab || ij \rangle$$

Compute eigenpairs of Hessian matrix.

If all eigenvalues are **positive**, we are at minima

If any eigenvalues are **negative**,  
lower energy solution exists.

What if we run into instability?

## Steepest Descent Method

1. Take the most **negative eigenvalue** and eigenvector
2. **Step wave function** in direction of eigenvector
3. **Re-optimize** GHF solution.

# Magnetic Materials

Full details and working equations in the paper!



$i, j, k, l$  refer to occupied orbitals,  $a, b, c, d$  refer to virtual orbitals, and  $p, q, r, s$  refer to any orbital. We also adopt Einstein summation, where the summation over common indices is implied. We begin with the Thouless representation of a single determinant. Thouless showed that any single Slater determinant can be transformed into another non-orthogonal single determinant via the transformation<sup>21</sup>

$$|\tilde{\phi}\rangle = e^{\hat{T}_1}|0\rangle, \quad (1)$$

where  $\hat{T}_1$  is a single particle excitation operator

$$\hat{T}_1 = \sum_{ia} t_i^a \{a_a^\dagger a_i\}. \quad (2)$$

In order to ensure that the Thouless transformation is enacted by a unitary transformation, we insist on the condition that  $\hat{T}_1$  is skew-Hermitian, i.e.,

$$\hat{T}_1 = -\hat{T}_1^\dagger \quad (3)$$

which implies that

$$t_i^a = -t_i^{a*}. \quad (4)$$

Consider the connected energy functional

$$E = \langle \tilde{\phi} | \hat{H}_N | \tilde{\phi} \rangle_c = \langle 0 | e^{\hat{T}_1^\dagger} \hat{H}_N e^{\hat{T}_1} | 0 \rangle_c, \quad (5)$$

where

$$\begin{aligned} \hat{H}_N &= \hat{H} - \langle 0 | \hat{H} | 0 \rangle = \hat{F}_N + \hat{V}_N = f_{pq} \{a_p^\dagger a_q\} \\ &\quad + \frac{1}{4} \langle pq || rs \rangle \{a_p^\dagger a_q^\dagger a_s a_r\} \end{aligned} \quad (6)$$

and  $\hat{H}$  is our Hamiltonian.  $\hat{F}_N$  and  $\hat{V}_N$  are the one- and two-body operators; the elements  $f_{pq}$  are the elements of the Fock matrix and  $\langle pq || rs \rangle$  are the antisymmetrized two electron integrals. For this parameterized functional, expanding through second order in  $\hat{T}_1$  gives

$$\begin{aligned} E &= \langle 0 | \hat{H}_N + \hat{T}_1^\dagger \hat{H}_N + \hat{H}_N \hat{T}_1 + \hat{T}_1^\dagger \hat{H}_N \hat{T}_1 + \frac{1}{2} \hat{T}_1^\dagger \hat{T}_1^\dagger \hat{H}_N \\ &\quad + \frac{1}{2} \hat{H}_N \hat{T}_1 \hat{T}_1 | 0 \rangle_c. \end{aligned} \quad (7)$$

Taking the first variation of  $E$  with respect to the Thouless parameters  $q_i^a = (t_i^a, t_i^{a*})$  about  $\hat{T}_1 = \hat{T}_1^\dagger = 0$ , gives

$$\frac{\partial E}{\partial q_i^a} = \begin{pmatrix} \langle \phi_i^a | \hat{H}_N | 0 \rangle_c \\ \langle 0 | \hat{H}_N | \phi_i^a \rangle_c \end{pmatrix} = \begin{pmatrix} f_{ia} \\ f_{ia} \end{pmatrix} \quad (8)$$

which must equal zero if the energy functional is minimized. Thus,  $f_{ia} = 0$  which are the off-diagonal elements of the Fock matrix, which is Brillouin's theorem. Taking the second variation of  $E$  with respect to the Thouless parameters yields

$$\frac{\partial^2 E}{\partial q_i^a \partial q_j^b} = \begin{pmatrix} \langle \phi_i^a | \hat{H}_N | \phi_j^b \rangle_c & \langle \phi_{ij}^{ab} | \hat{H}_N | 0 \rangle_c \\ \langle 0 | \hat{H}_N | \phi_{ij}^{ab} \rangle_c & \langle \phi_j^b | \hat{H}_N | \phi_i^a \rangle_c \end{pmatrix}. \quad (9)$$

For the Hartree-Fock equations to be stable, the second variation must be positive semidefinite, i.e.,  $\delta^{(2)}E \geq 0$ . Putting the second variation in matrix form, we obtain the Hessian

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{pmatrix}, \quad (10)$$

where

$$A_{ia,jb} = (\epsilon_a - \epsilon_i) \delta_{ia,jb} + \langle aj || ib \rangle, \quad B_{ia,jb} = \langle ab || ij \rangle. \quad (11)$$

For the complex GHF equations, the orbital energies will be real as they are the eigenvalues of a Hermitian matrix. The antisymmetrized two-electron integrals, however, will be complex. Thus, in the complex GHF case,  $\mathbf{A} \neq \mathbf{A}^*$  and  $\mathbf{B} \neq \mathbf{B}^*$ . At any stationary solution to the Hartree-Fock equations, the above Hessian may be constructed and diagonalized. Strictly negative eigenvalues indicate an instability, and the corresponding eigenvector indicates the direction in which the Hartree-Fock energy will decrease. This can be accomplished by taking the eigenvector corresponding to the lowest eigenvalue (steepest descent) and constructing a complex-valued ( $2N \times 2N$ ) mixing matrix  $\mathbf{K}$ , where  $N$  is the number of basis functions,<sup>1</sup>

$$\mathbf{K} = \begin{pmatrix} \mathbf{0} & -\mathbf{J}^\dagger \\ \mathbf{J} & \mathbf{0} \end{pmatrix}, \quad (12)$$

where  $\mathbf{J}$  is the ( $O \times V$ ) eigenvector corresponding to the lowest eigenvalue. This mixing matrix is exponentiated to give the unitary rotation matrix that transforms the old set of MO coefficients  $\mathbf{C}$  to a new set of rotated MO coefficients  $\mathbf{C}'$ ,

$$\mathbf{C}' = \mathbf{C} e^{-s\mathbf{K}}, \quad (13)$$

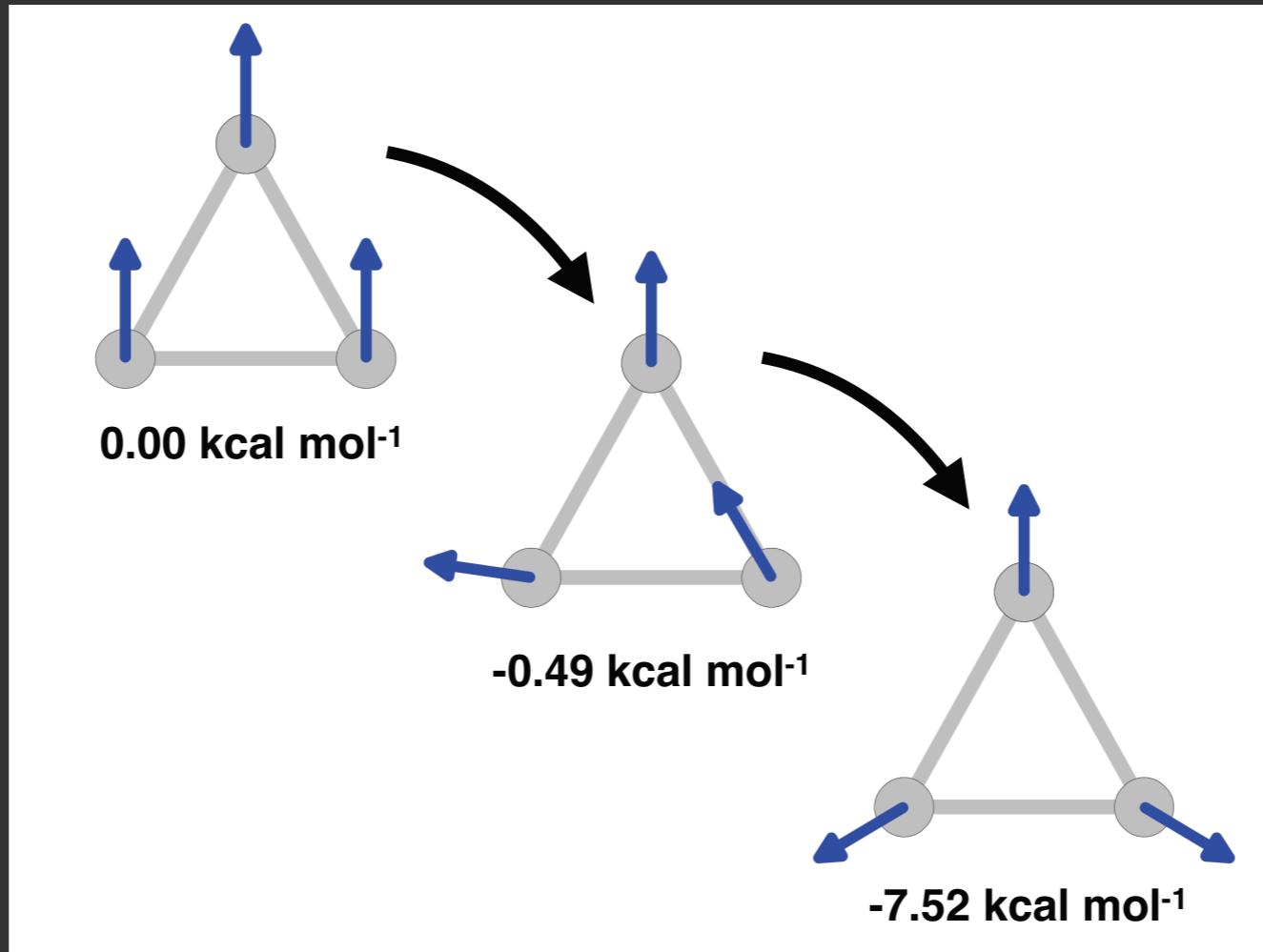
where  $s$  is some small step in the direction  $\mathbf{K}$ . The new rotated MO coefficients may be fed back into the SCF procedure and the Hartree-Fock solutions re-optimized. With a suitable step-size, the Hartree-Fock equations will converge to a lower energy solution, and the stability test may be performed again.

### III. DISCUSSION

Among the first row elements, GHF solutions are rare. However, molecular systems involving geometric frustration are prime targets for a GHF analysis because their frustrated spins must break  $\hat{S}_z$  symmetry in order to minimize Pauli repulsion. Geometrically frustrated systems have long been a target for GHF and noncollinear DFT methods.<sup>7–14</sup> Thus, to explore the applicability of our GHF stability tests, we examined a series of neutral hydrogen rings, ranging from 3 to 15 hydrogens. Each hydrogen was spaced 1 Å around a circle. The advantage of studying such a system is threefold: first, the system is simple enough that we can be guided by chemical intuition, second, at such a spacing, the hydrogen rings act similar to 1D hydrogen chains that prefer an antiferromagnetic alignment, and third, each odd-membered ring will be geometrically frustrated. There are few studies of hydrogen rings,<sup>22,23</sup> but this appears to be the first to study the geometrically frustrated neutral, odd-numbered hydrogen rings. This geometric frustration means that a GHF solution must exist which minimizes the repulsion from the frustrated spin alignment. It bears mentioning that although the system appears to be artificial, equilateral  $H_3^+$  is among one of the most common ions in interstellar gases,<sup>24,25</sup> and  $H_3$  has been observed experimentally.<sup>26</sup> Furthermore, recent combined theoretical/experimental reports have demonstrated the evidence of sigma-aromatic  $H_5^-$  when

# Magnetic Materials

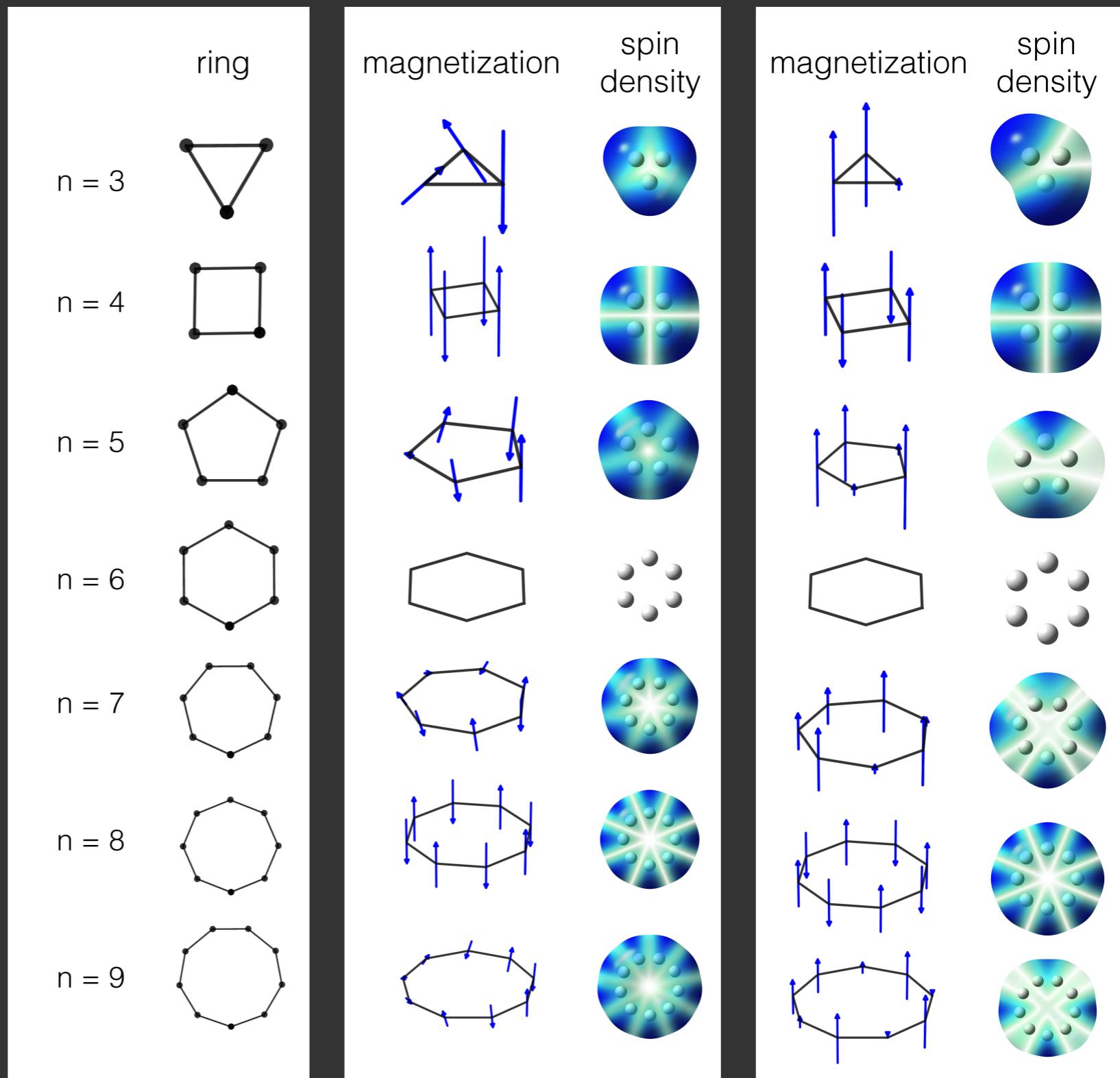
Looking for lowest energy solutions  
in spin frustrated rings



Cr<sub>3</sub> : high-spin solutions unstable.  
Lower energy non-collinear solution exists.

# Magnetic Materials

Hydrogen rings  
for odd-member  
rings, GHF  
lowest energy  
solution



# Magnetic Materials

## In summary:

GHF allows for the **lowest-energy HF solution**

Can **determine multiplicity** without user input

Can **handle spin frustrated** systems

Loses all good **spin quantum numbers**

## Future outlook

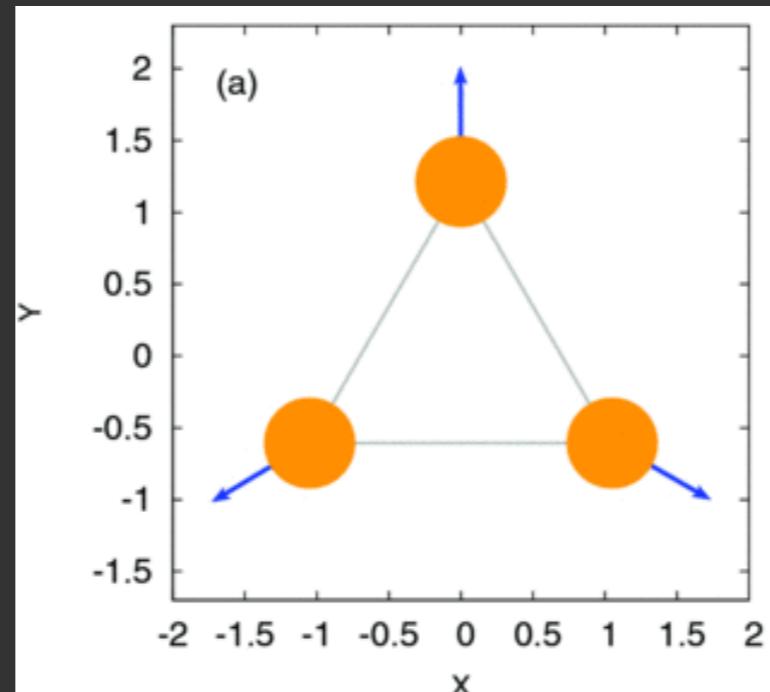
GHF can handle spin transitions,  
but **lacks any spin operators**  
(only Coulomb exchange interaction)

# Including Arbitrary Magnetic Fields into *Ab Initio* Electron Dynamics

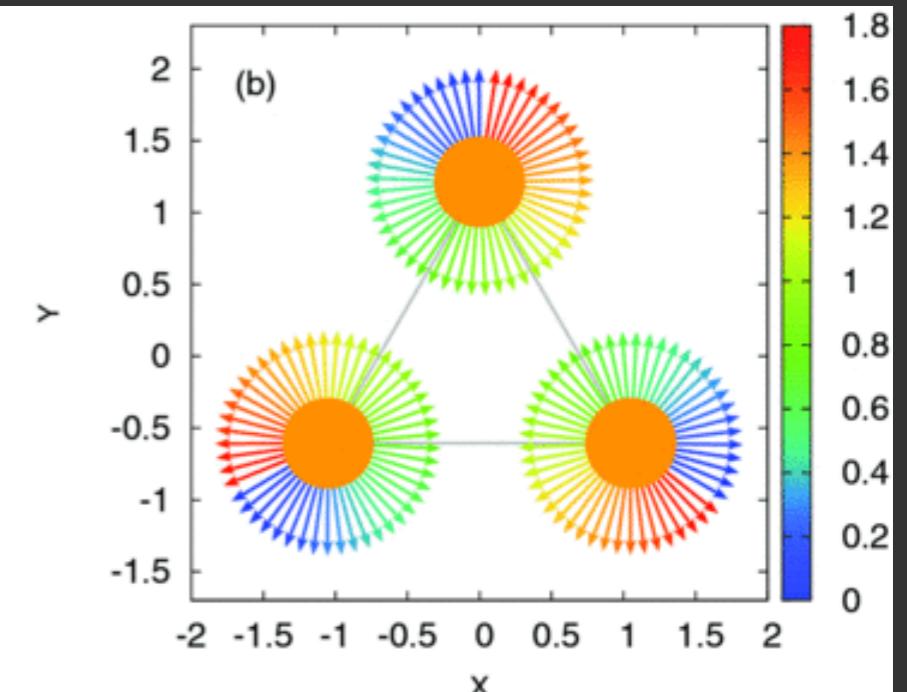
## RT-TD-GHF

- Arbitrary magnetic field
- Magnetic moments precess with field
- No spin coupling!

## Initial Magnetization



## Time Evolution (ps)



Neutral Li<sub>3</sub> trimer, 20T field perpendicular to plane

**Observation: TD-GHF allows smooth evolution of spin states, but lacks spin coupling operators**

**Can we extend this description by adding explicit spin operators to the TD-GHF description?**

**Spin is a non-classical effect.  
It arises from relativistic quantum mechanics.**

**One electron, Dirac equation:**

$$\begin{bmatrix} V & c\boldsymbol{\sigma} \cdot \boldsymbol{\Pi} \\ c\boldsymbol{\sigma} \cdot \boldsymbol{\Pi} & V - 2c^2 \end{bmatrix} \begin{bmatrix} \Psi^L \\ \Psi^S \end{bmatrix} = E \begin{bmatrix} \Psi^L \\ \Psi^S \end{bmatrix}$$

**This replaces the one electron operators in GHF**

**Note four component:**

$$\Psi^L = \begin{bmatrix} \Psi^{L\alpha} \\ \Psi^{L\beta} \end{bmatrix} \quad \Psi^S = \begin{bmatrix} \Psi^{S\alpha} \\ \Psi^{S\beta} \end{bmatrix}$$

**For multiple electrons, we have the approximate interaction operator—the Breit operator**

$$\hat{V}_{12} = \frac{q_1 q_2}{r_{12}} - \frac{q_1 q_2}{2} \left[ \frac{\alpha_1 \cdot \alpha_2}{r_{12}} + \frac{(r_{12} \cdot \alpha_1)(r_{12} \cdot \alpha_2)}{r_{12}^3} \right]$$

**This replaces the two electron Coulomb operator**

$$\alpha = \begin{pmatrix} 0_2 & \sigma \\ \sigma & 0_2 \end{pmatrix}$$

**For multiple electrons, we have the approximate interaction operator—the Breit operator**

$$\hat{V}_{12} = \frac{q_1 q_2}{r_{12}} - \frac{q_1 q_2}{2} \left[ \frac{\alpha_1 \cdot \alpha_2}{r_{12}} + \frac{(r_{12} \cdot \alpha_1)(r_{12} \cdot \alpha_2)}{r_{12}^3} \right]$$

(Coulomb)

(Breit correction, note spin-dependence)

This replaces the two electron Coulomb operator

$$\alpha = \begin{pmatrix} 0_2 & \sigma \\ \sigma & 0_2 \end{pmatrix}$$

We can reduce to two component form

$$\begin{bmatrix} H_{LL} & H_{LS} \\ H_{SL} & H_{SS} \end{bmatrix} \begin{bmatrix} \Psi^L \\ \Psi^S \end{bmatrix}$$

$$U \begin{bmatrix} H_{LL} & H_{LS} \\ H_{SL} & H_{SS} \end{bmatrix} U^{-1} \rightarrow \begin{bmatrix} \tilde{H}_{LL} & 0 \\ 0 & \tilde{H}_{SS} \end{bmatrix}$$

Usually approximate

Off diagonal terms zero to some order

Order 1/c gives Breit-Pauli

Order V gives Douglas-Kroll-Hess

$$\Psi^L = \begin{bmatrix} \Psi^{L\alpha} \\ \Psi^{L\beta} \end{bmatrix}$$

$$\Psi^S = \begin{bmatrix} \Psi^{S\alpha} \\ \Psi^{S\beta} \end{bmatrix}$$

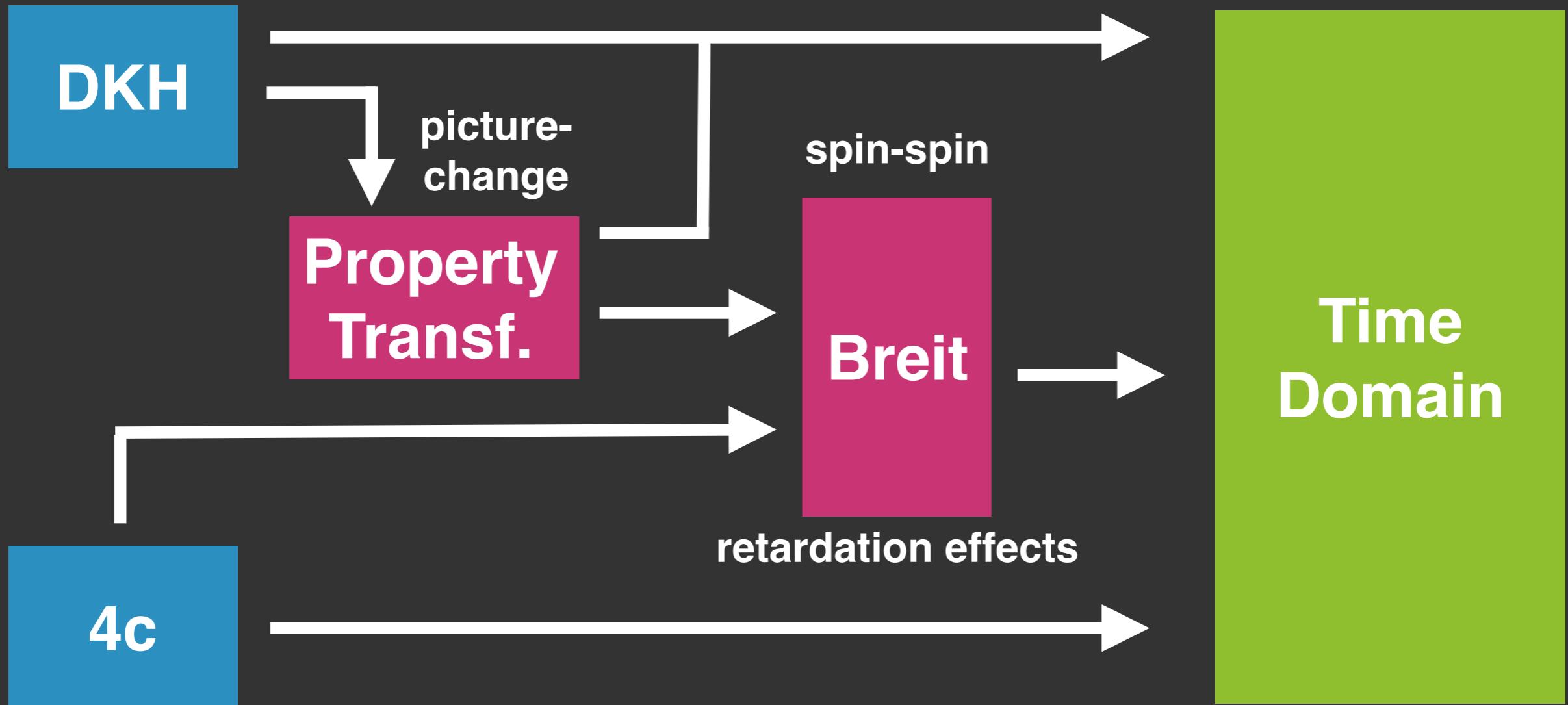
# Uncertain best way to include these operators into the TDSE

	<b>Four Component</b>	<b>Breit-Pauli (two component, 1/c)</b>	<b>Douglas-Kroll- Hess (two component,V)</b>
<b>Naive cost?</b>	$2(4N)^4$	$2(2N)^4$	$2(2N)^4$
<b>Variational?</b>	No (yes, in practice)	No	Yes
<b>Interpretation?</b>	Must account for positron-like component	Clear relation to spin-Hamiltonian	Spin-terms mixed

# Future Roadmap

cheaper,  
harder to code

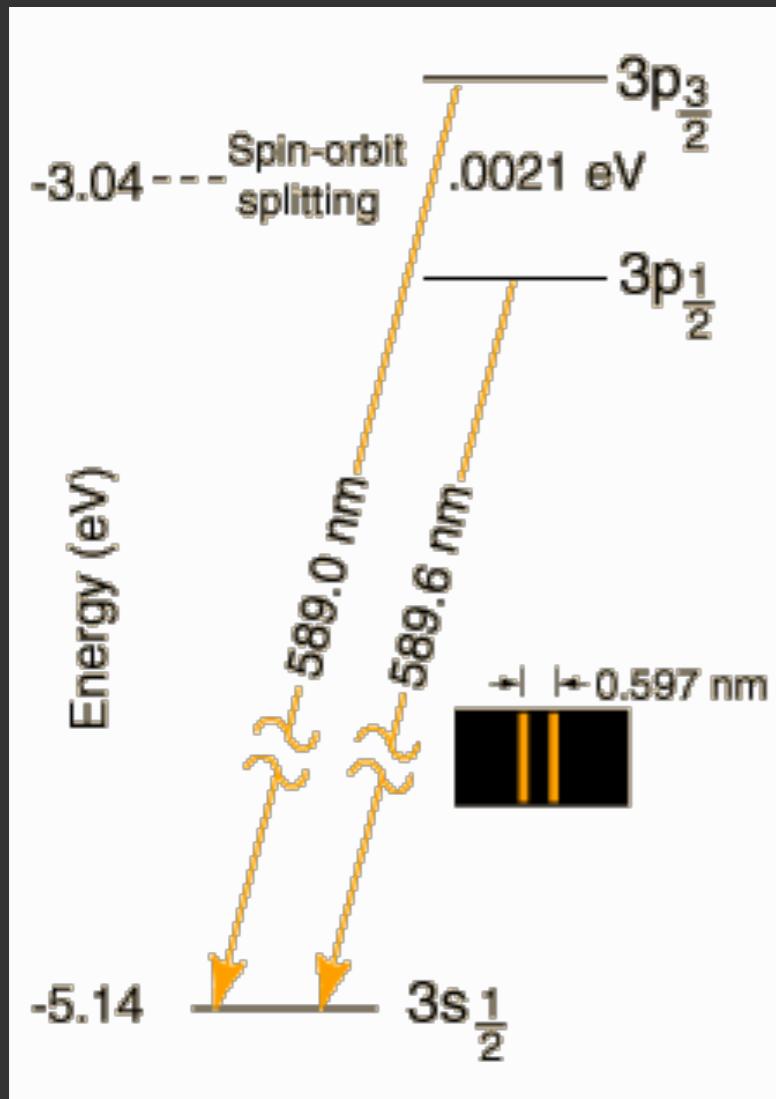
response properties,  
physical observables



Spin-dependent electronic dynamics  
Heavy-element response properties

**How can we predict and understand  
the electronic and magnetic responses  
of molecules and nano-materials?**

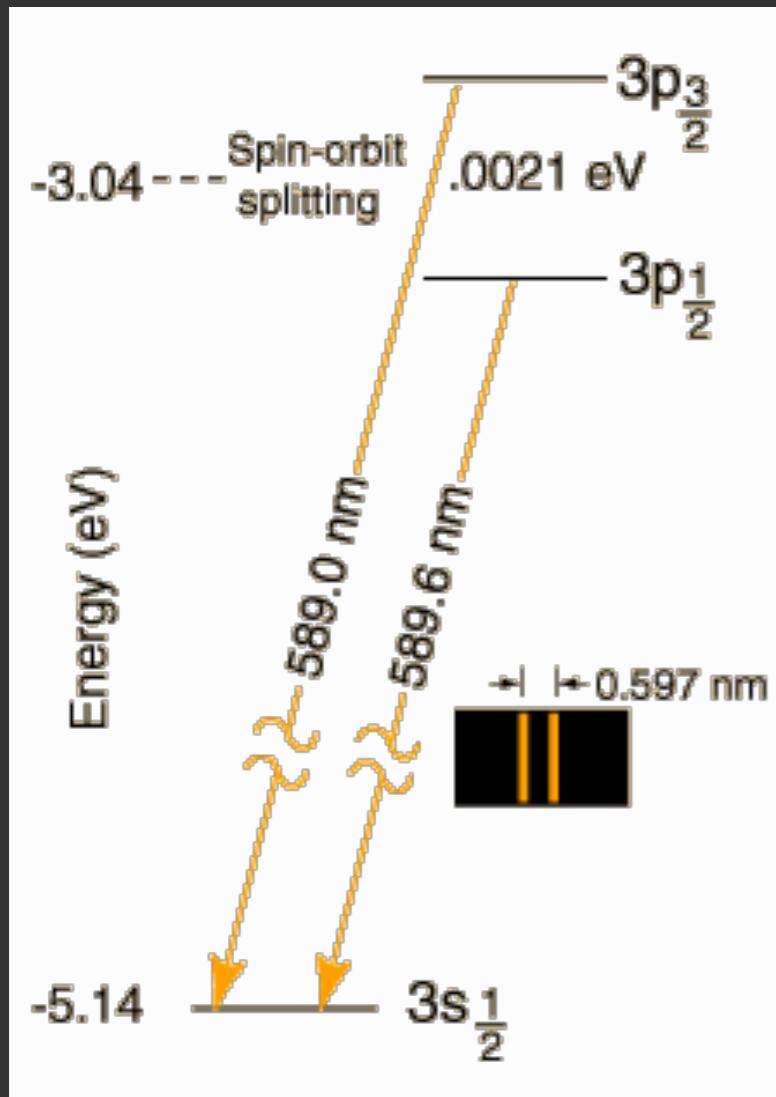
# Maybe settle for atoms at the moment?



## TD-DKH Sodium D-lines (daug-cc-pVTZ)

[eV]	1c-TD-DKH	2c-TD-DKH	Exp
$^2S_{1/2} \rightarrow ^2P_{1/2}$	<b>1.9733</b>	<b>1.9730</b>	<b>2.1023</b>
$^2S_{1/2} \rightarrow ^2P_{3/2}$	<b>1.9733</b>	<b>1.9736</b>	<b>2.1044</b>
Splitting	0.0000	0.0006	0.0021

# Maybe settle for atoms at the moment?



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<b>Splitting</b>	<b>0.0000</b>	<b>0.0006</b>	<b>0.0021</b>

A lot more more needs to be done!

## Future work



**Spin-dependent dynamics  
and response theory**

## Future work



Spin in Time-  
Dependent  
Theory

**Spin-dependent dynamics  
and response theory**

**Thank you!**

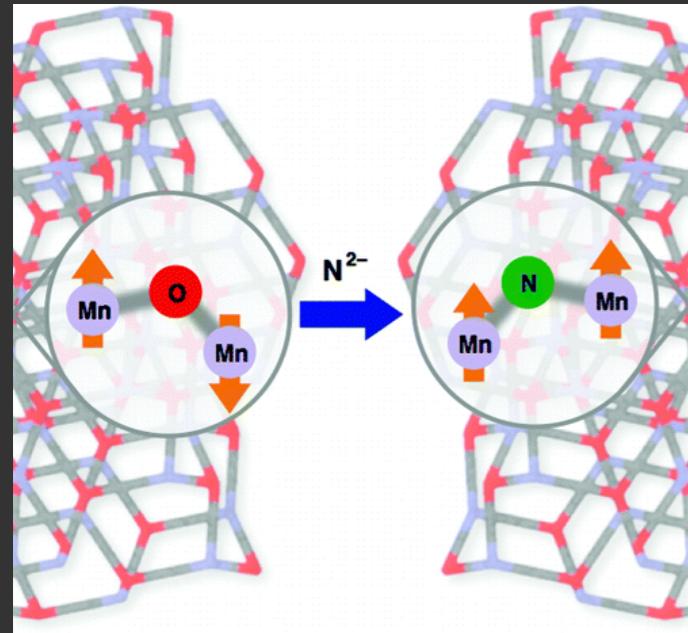
**Li Group  
Exam Committee  
Ernest Davidson**





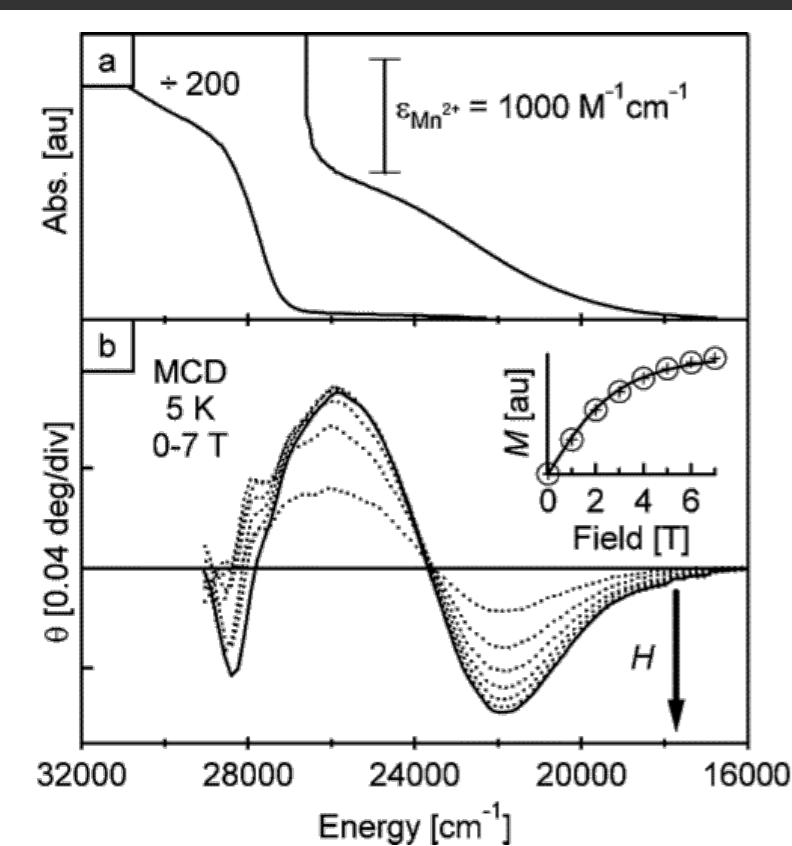


# Coupling between charge carriers and Mn<sup>2+</sup> in ZnO QDs



holes in p-type dopants couple with Mn<sup>2+</sup> dimer

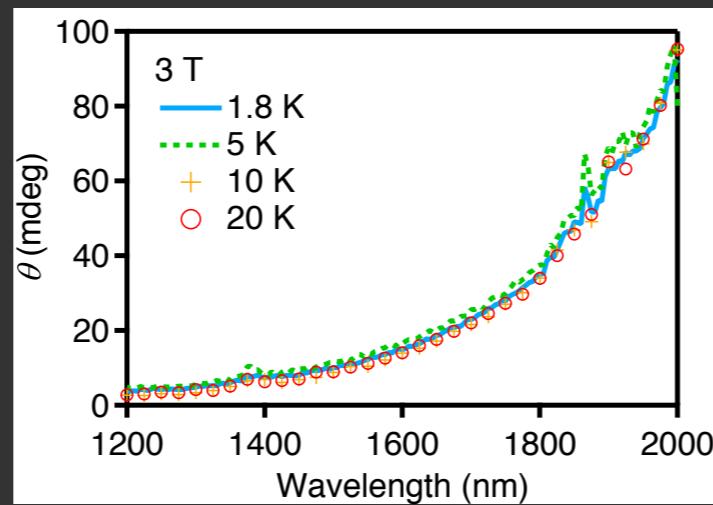
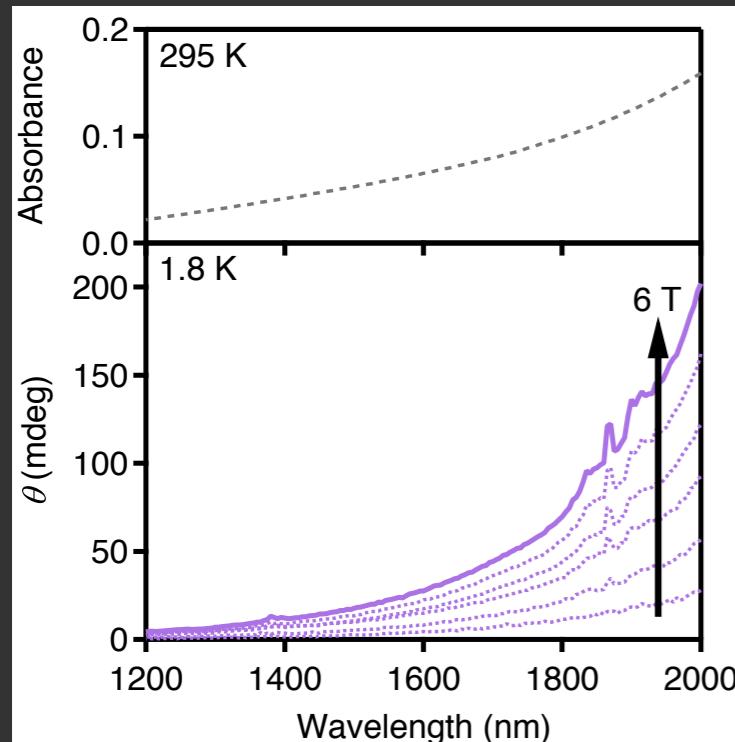
May, Joseph W., Ryan J. McMorris, and Xiaosong Li. *JPCL*  
3.10 (2012): 1374-1380.



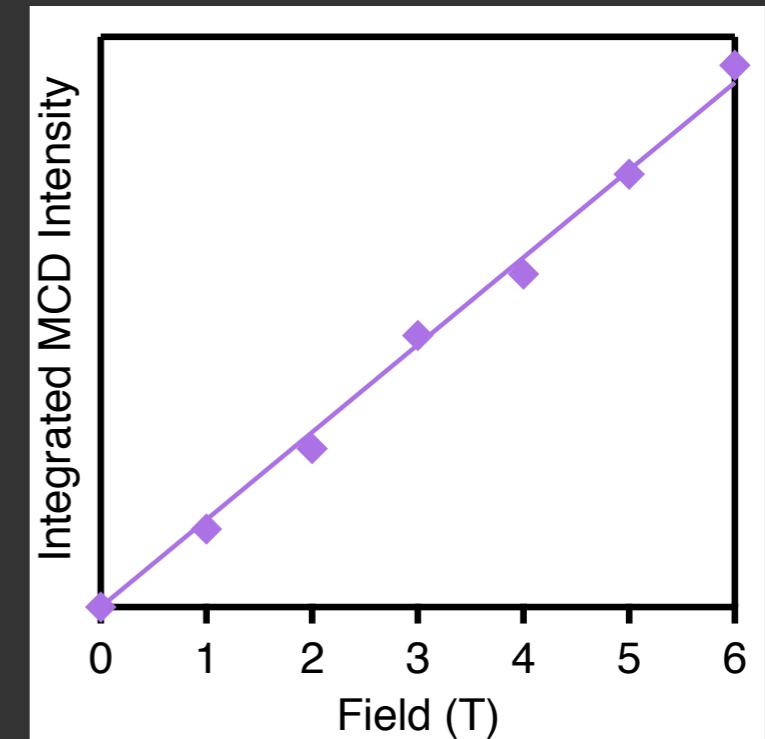
exciton couples to Mn<sup>2+</sup> in ZnO QDs

Norberg, Nick S., et al. *JACS* 126.30 (2004): 9387-9398.

It seems reasonable that excess CB electrons would couple to Mn



Data courtesy  
Dr. Alina Schimpf

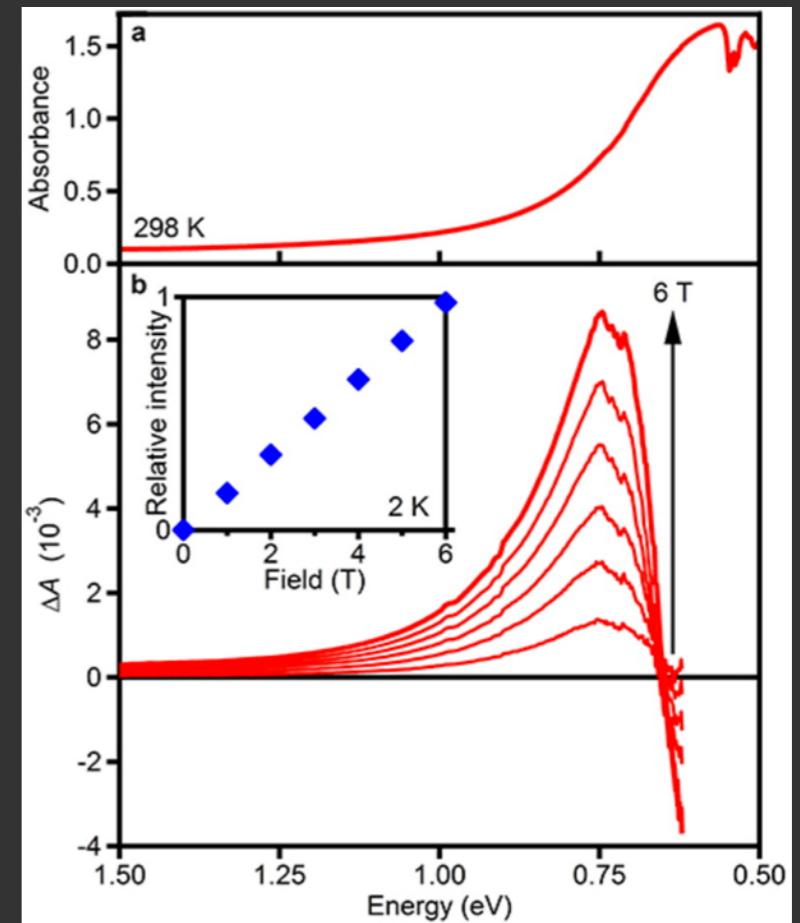


Al<sup>3+</sup>:ZnO QDs; no evidence excess electrons couple with Mn

Of course, similar story with photodoped e<sup>-</sup>:ZnO

All systems studied so far are heavily doped

Currently, Gamelin group looking at low-carrier concentrations



Schimpf, A. M., Thakkar, N., Gunthardt, C. E., Masiello, D. J., & Gamelin, D. R. (2013). ACS Nano, 8(1), 1065-1072.

Can we help explain this with spin dependent electronic structure theory?