Session T72: New Approaches for Spins and Emitters

Show Abstracts

Focus

Sponsoring Units: DMP
Room: *Hyatt Regency Hotel -Jackson Park D*

Thursday, March 17, 2022 11:30AM - 12:06PM	T72.00001: Active Space Wavefunction Methods for Defects in Solids Invited Speaker: John P Philbin
Thursday, March 17, 2022 12:06PM - 12:18PM	T72.00002: Extrinsic and Intrinsic Defects in MgO and CaO as potential spin-qubit candidates Christian W Vorwerk, Nan Sheng, Marco Govoni, Giulia Galli
Thursday, March 17, 2022 12:18PM - 12:30PM	T72.00003: Efficient Characterization of Features in Micro-Photoluminescence Images for the Identification of Single-Photon Emitters Leah Narun, Rebecca Fishman, Henry Shulevitz, Raj Patel, Lee Bassett
Thursday, March 17, 2022 12:30PM - 1:06PM	T72.00004: Emerging rare-earth doped materials for quantum information Invited Speaker: Elizabeth A Goldschmidt
Thursday, March 17, 2022 1:06PM - 1:18PM	T72.00005: Terahertz nano-imaging of heterogeneous dipole fields and charge scattering at a single nanojunction Samuel J Haeuser, Richard Kim, Joongmok Park, Lin Zhou, Matthew J Kramer, Mark Field, Cameron J Kopas, Josh Y Mutus, Jin-Su Oh, Jigang Wang
Thursday, March 17, 2022 1:18PM - 1:30PM	T72.00006: Instability of rock-salt cubic NbN in density functional calculations Anuj Goyal, Sage Bauers, Stephan Lany
Thursday, March 17, 2022 1:30PM - 1:42PM	T72.00007: Si-integrated $BaTiO_3$ modulators for Quantum Computing with Si photonics Alexander A Demkov, Agham Posadas, Daniel Wassertman, Zuoming Dong
Thursday, March 17, 2022 1:42PM - 1:54PM	T72.00008: Modeling the Optical Properties of Hidden Silicon-Vacancy Centers in Diamond Tommy Wen J Chin, Christopher L Smallwood
Thursday, March 17, 2022 1:54PM - 2:06PM	T72.00009: Experimental and Computational Investigations of Boron-Nitrogen Pairs in Diamond for Quantum Information Applications Anil Bilgin, Jeremy Estes, Ian N Hammock, Hannes Bernien, Alexander A High, Giulia Galli
Thursday, March 17, 2022 2:06PM - 2:18PM	T72.00010: Beryllium oxide as a host for quantum defects YUBI CHEN, Mark E Turiansky, Chris G Van de Walle
Thursday, March 17, 2022 2:18PM - 2:30PM	T72.00011: Decoherence of nitrogen-vacancy spin ensembles in diamond in the nitrogen electron-nuclear spin bath Huijin Park, Junghyun Lee, Sangwook Han, Sangwon Oh, Hosung Seo

Extrinsic and Intrinsic Defects in MgO and CaO as Potential Spin-Qubit Candidates

Christian Vorwerk[1], Nan Sheng[2], Marco Govoni[3], and Giulia Galli[1,3]

[1] Pritzker School of Molecular Engineering, University of Chicago.
[2] Department of Chemistry, University of Chicago, Chicago.
[3] Materials Science Division and Center for Molecular Engineering, Argonne National Laboratory.

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MICCoM

MgO and CaO as Qubit Host Materials: Excellent Spin Coherence Time

Estimated spin coherence time T_2

#	Material	T_2 (ms)	#	Material	T_2 (ms)	#	Material	T_2 (ms)
1	CeO_2	47	12	CaS	23	23	WS_2	11
2	FeO	36	13	Ca_2NiWO_6	19	24	$Sr_2Si(S_2O_7)_4$	11
3	CaO	34	14	S	19	25	$Sr_2Ge(S_2O_7)_4$	11
4	$CaSO_4$	29	15	$CaWO_4$	18	26	$CaCO_3$	11
5	$Ce(SO_4)_2$	29	16	CS_{14}	18	27	FeS_2	10
6	SO_3	29	17	Fe_2NiO_4	18			
7	$FeSO_4$	28	18	S_8O	17	138	SiO_2	2.7
8	CaS_3O_{10}	28	19	$FeWO_4$	16	298	ZnO	1.9
9	Ca_3WO_6	27	20	$NiSO_4$	15	709	SiC	1.1
10	WS_2O_9	25	21	WO_3	13	936	diamond	0.89
11	Ca_2FeWO_6	24	22	$NiWO_4$	12	1125	MgO	0.60

S. Kanai et al., preprint arXiv:2102.02986 (2021).

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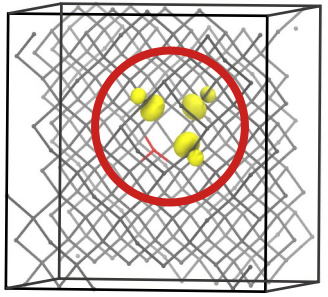
What are suitable defects in MgO and CaO ?

Electronic Structure of Defects from First Principles

Initial guess of suitable defects



Identify set of localized defect orbitals

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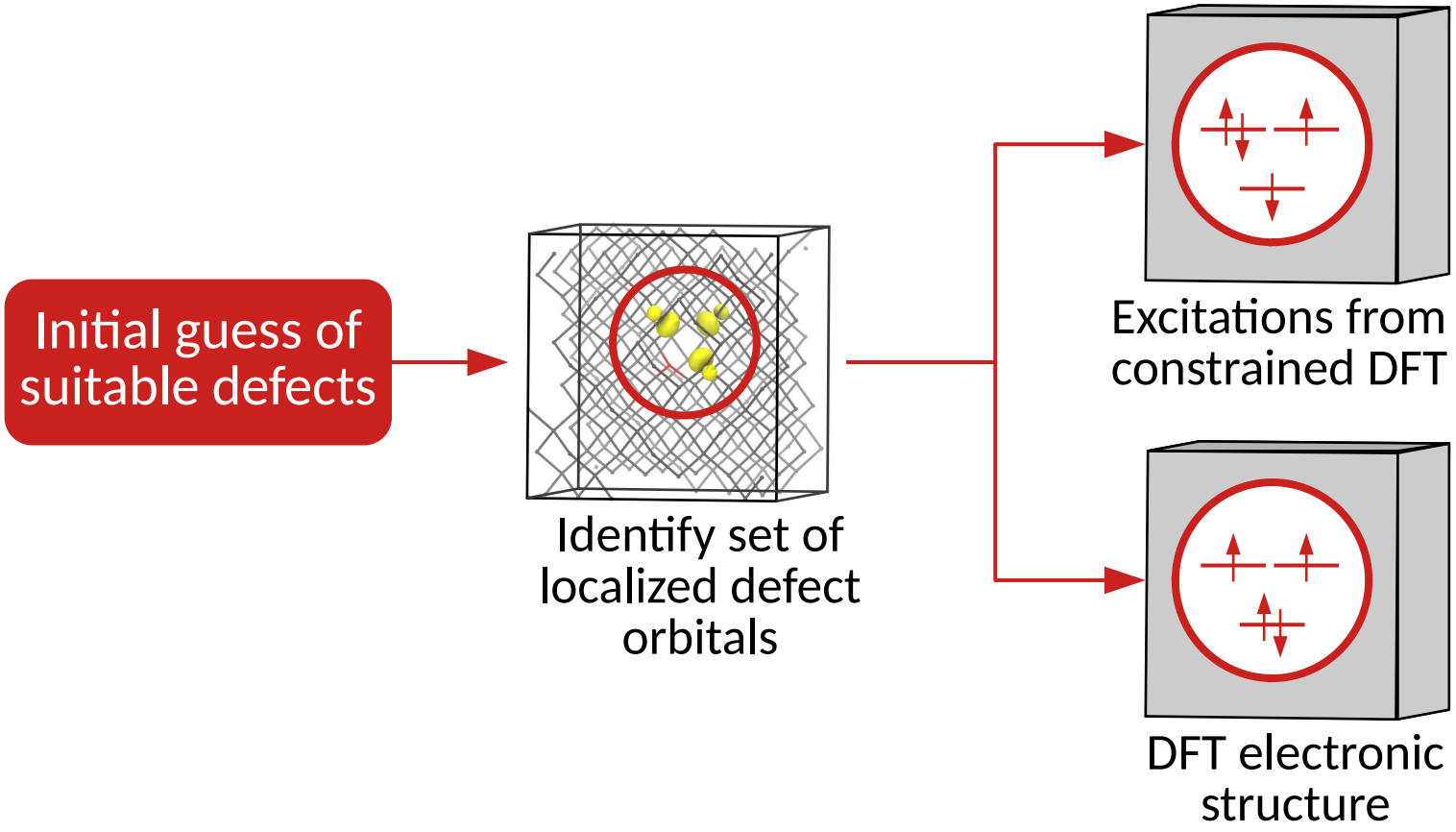

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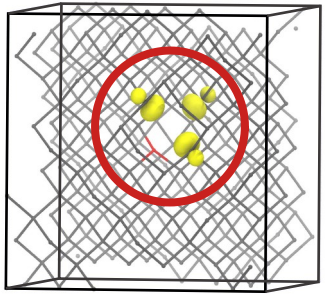

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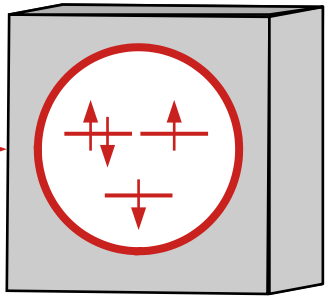
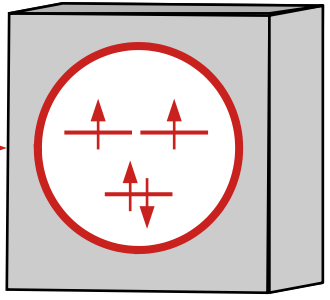


Excitations from constrained DFT

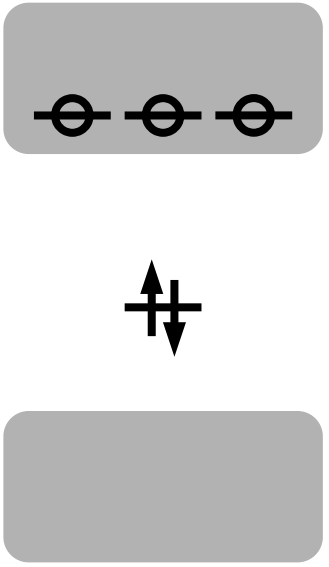


DFT electronic structure

- Quantum Espresso Calculations
- Γ-centered 2x2x2 supercell
- SG15 ONCV pseudo-potentials
- PBE functional

Intrinsic Point Defects

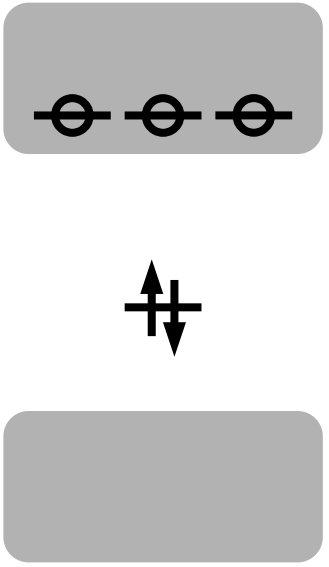
Oxygen Vacancy



- S=0 groundstate
- No excitations within band gap

Intrinsic Defects in MgO

Oxygen Vacancy



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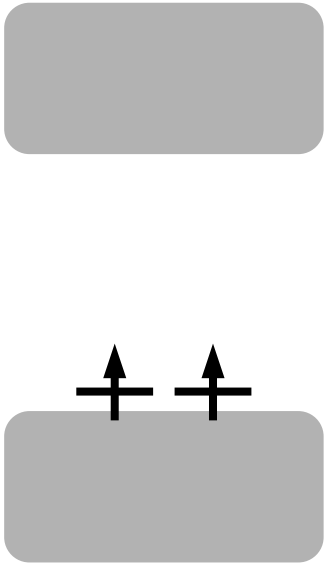
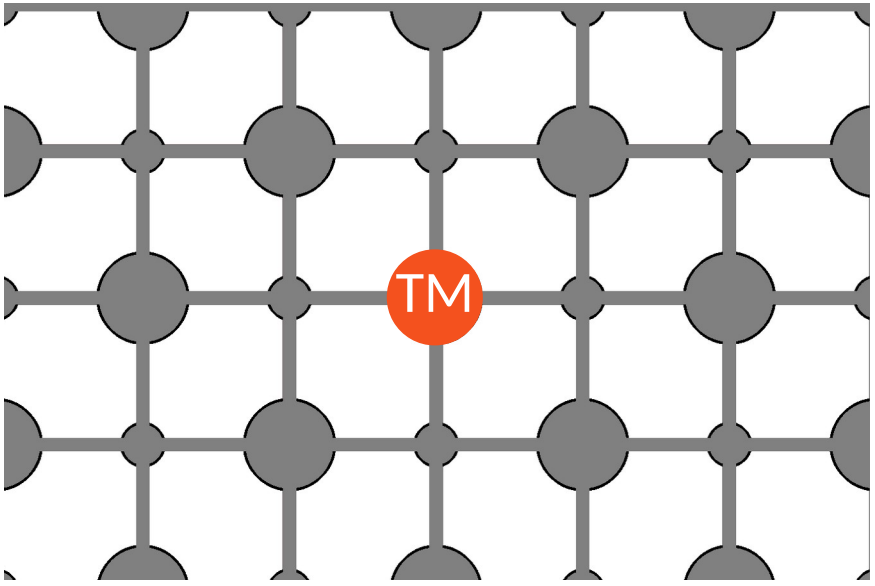
Magnesium/Calcium Vacancy



- S=1 groundstate
- No unoccupied defect orbital
- Only ionization possible

Exctrinsic Defects: Transition-Metal Doping



Ni_{Mg}^{0}: [Ar]$3d^{8}$ $4s^{0}$

Pt_{Mg}^{0}: [Xe]$4f^{14}$ $5d^{8}$ $6s^{0}$

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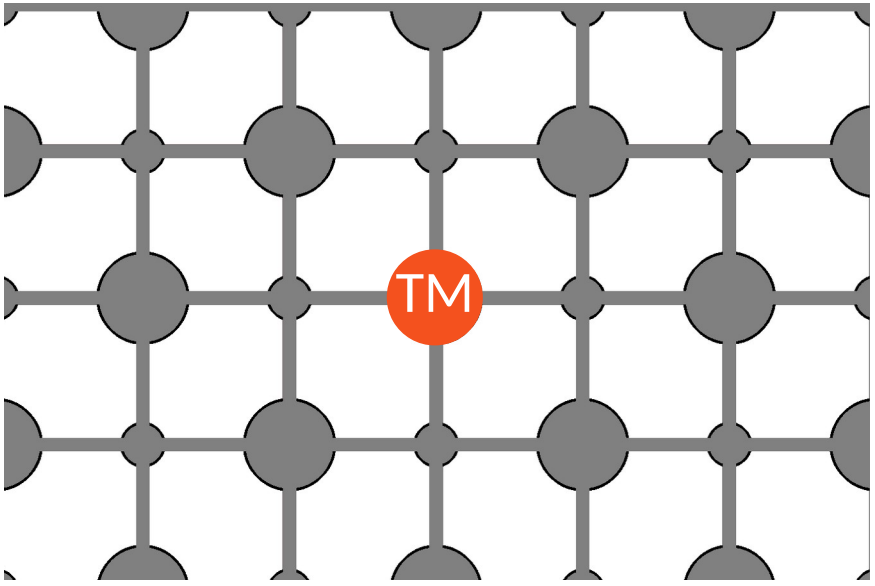

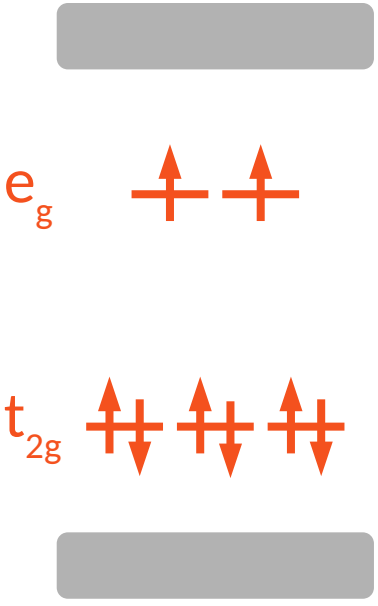

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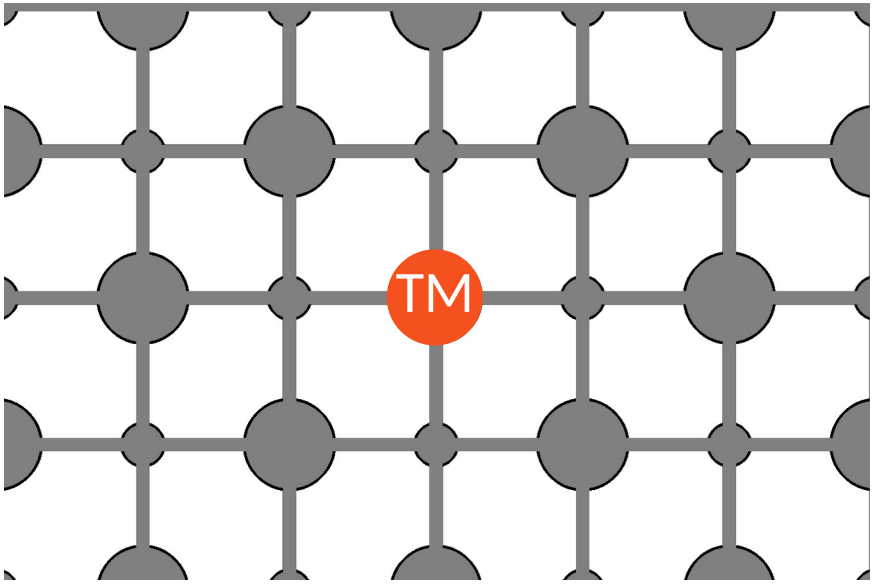

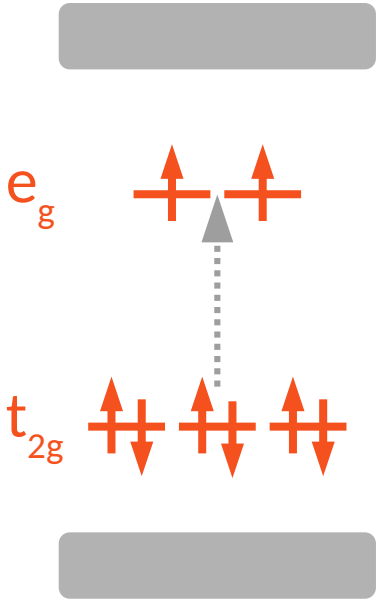

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Transition-Metal Defects: Absorption Energies (Zero-phonon Lines)

	cDFT [eV]	Exp. Ref. [eV]	Theo. Ref. [eV]
Ni:MgO	1.20 (1.18)	1.00[1] (0.97)[2]	0.84 (0.73)[3]
Pt:MgO	2.31 (2.26)		2.70 (2.51)[4]
Ni:CaO	0.56 (0.54)		
Pt:CaO	1.45 (1.40)		1.87 (1.71)[4]

1 J.E. Ralph and M.G. Townsend, J. Phys. C: Solid State Phys. **3**, 8 (1970).
2 S.A. Payne, Phys. Rev. B **41**, 6109 (1990).
3 G.D. Cheng, L. Yan, and Y. Chen, J. Mater. Sci. **52**, 8200 (2017).
4 C. Zhou, Z. Li, and J. Yang, Comput. Mater. Sci. **181**, 109754 (2020).

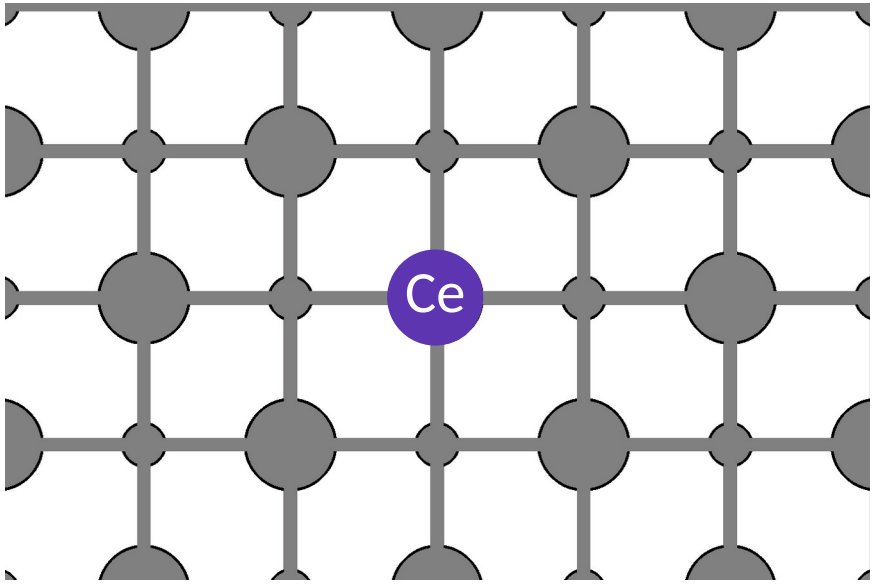
Transition-Metal Defects: Radiative Lifetimes

Radiative rate: $$\Gamma = \frac{n_D \mathbf{P}^2 E_{\mathrm{ZPL}}^3 e^2}{3\pi\epsilon_0 c^3 \hbar^4}$$

	DFT
Ni:MgO	5183 s
Pt:MgO	648 s
Ni:CaO	9 s
Pt:CaO	5 s
NV^-:Diamond	14 ns

Decreasing lifetime with increasing Z and decreasing band gap

Exctrinsic Defects: Lanthanide Defects



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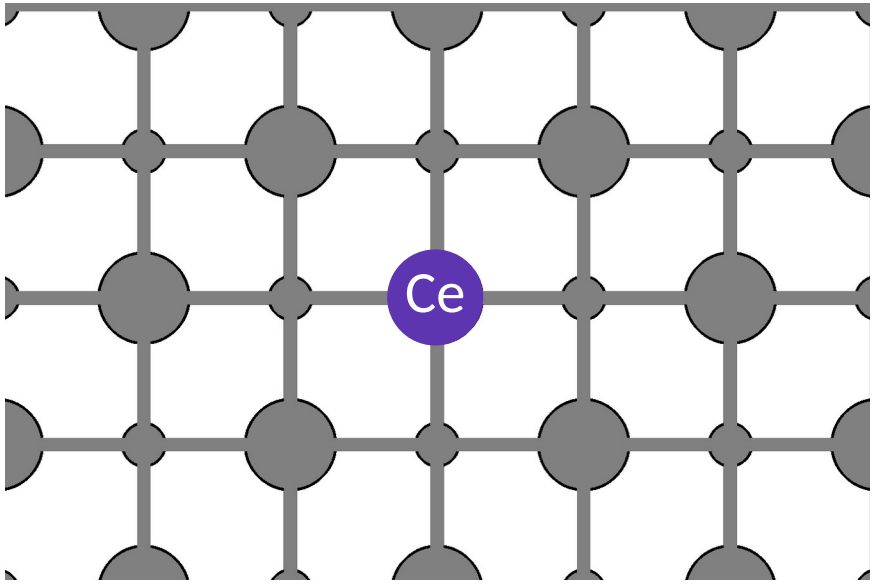

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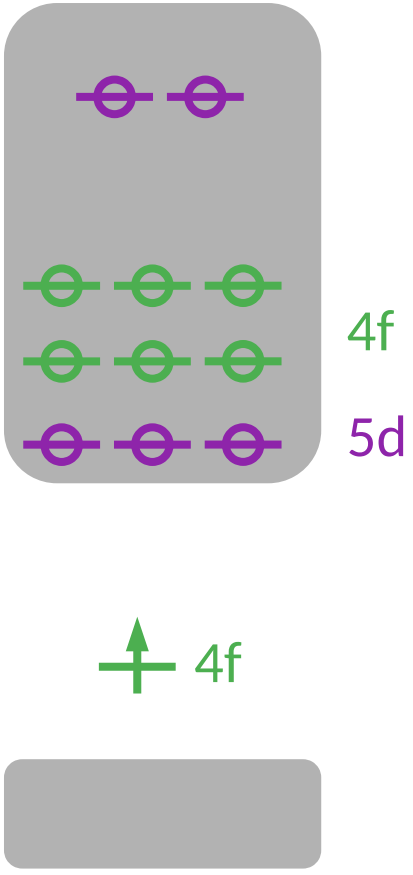

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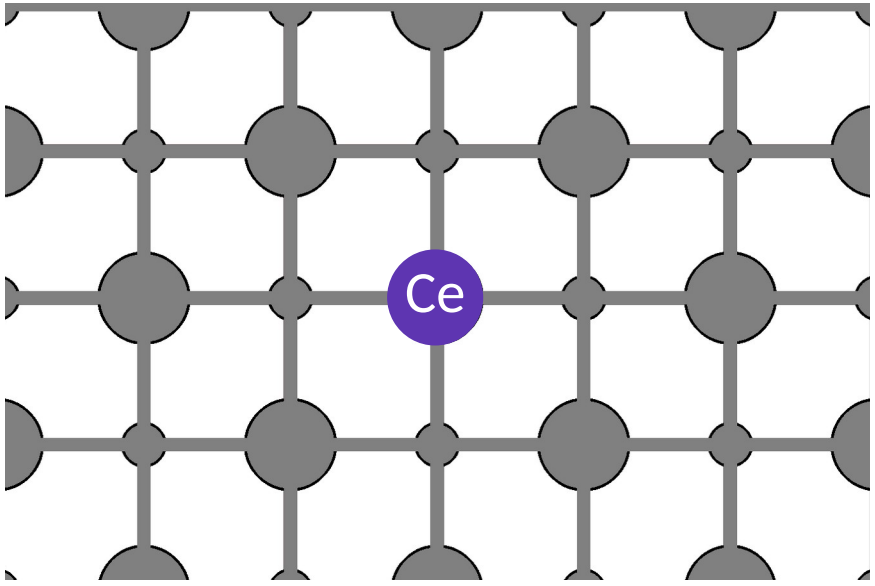

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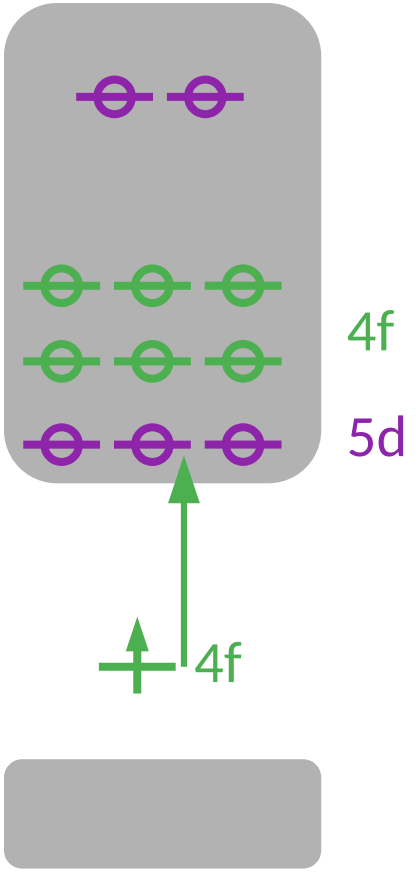

Hubbard Corrections for Localized Ce *4f* States

Localized *4f* orbitals not well described within DFT → DFT+U yields corrections

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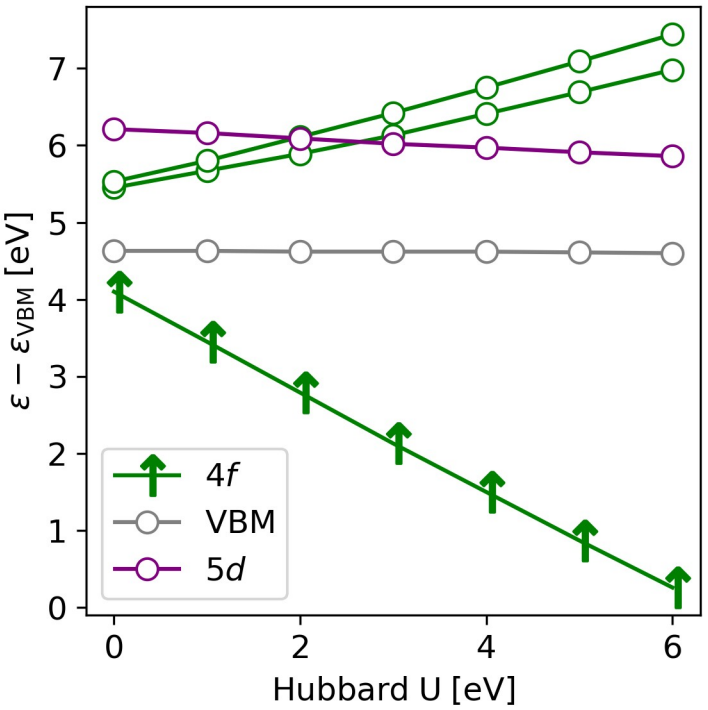

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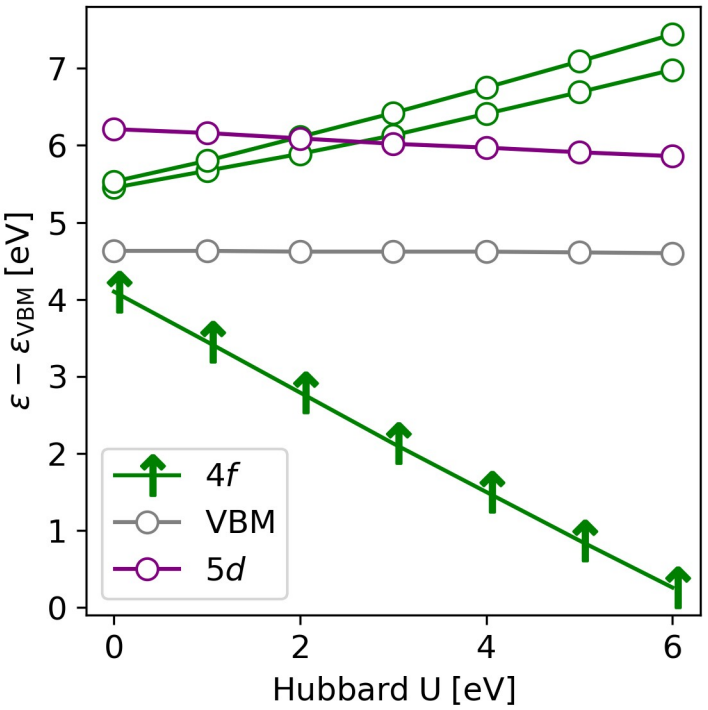

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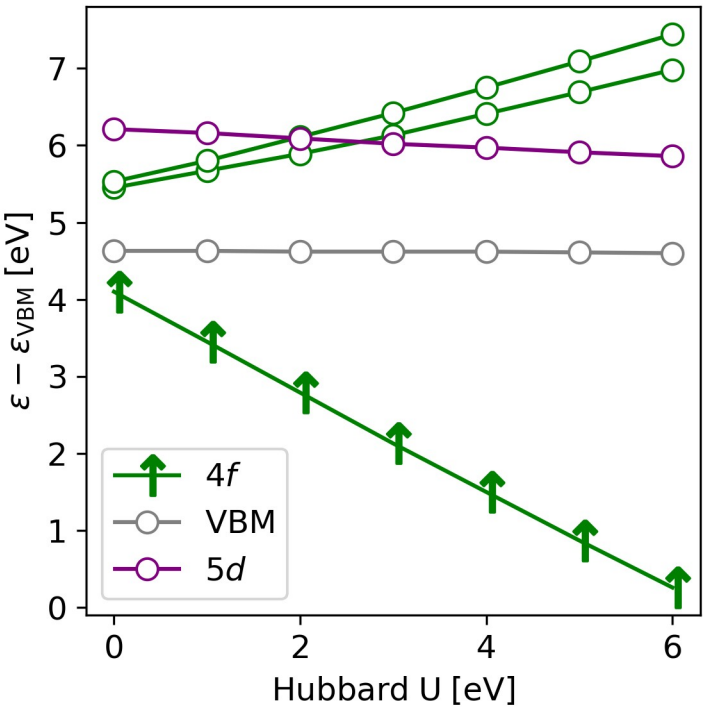

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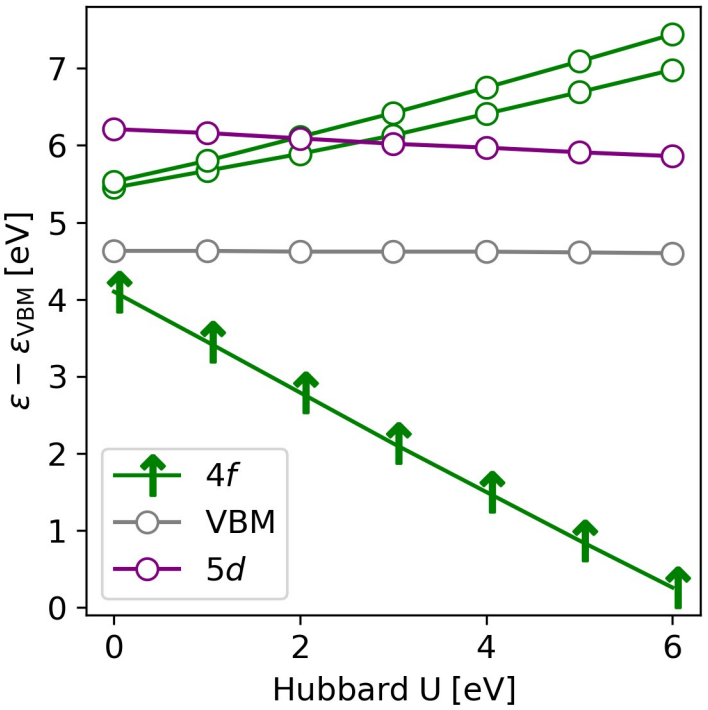

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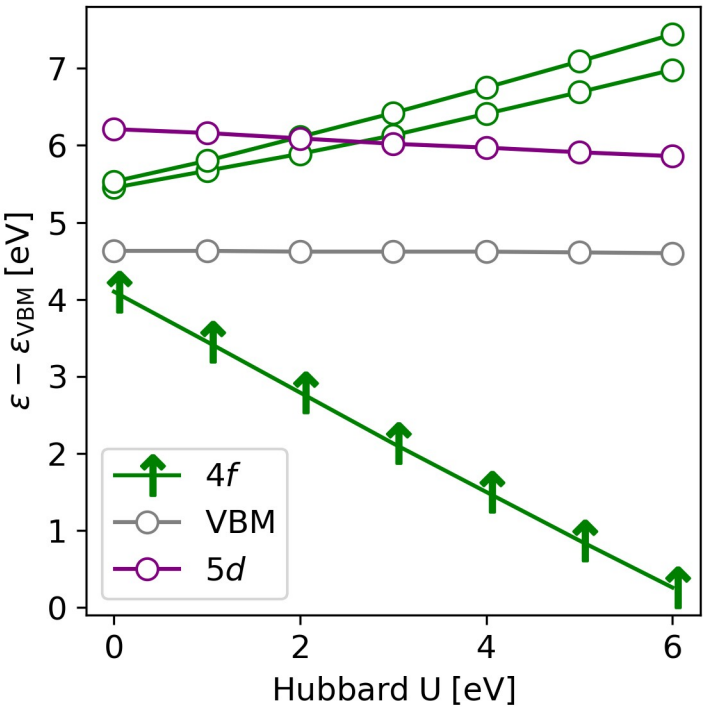

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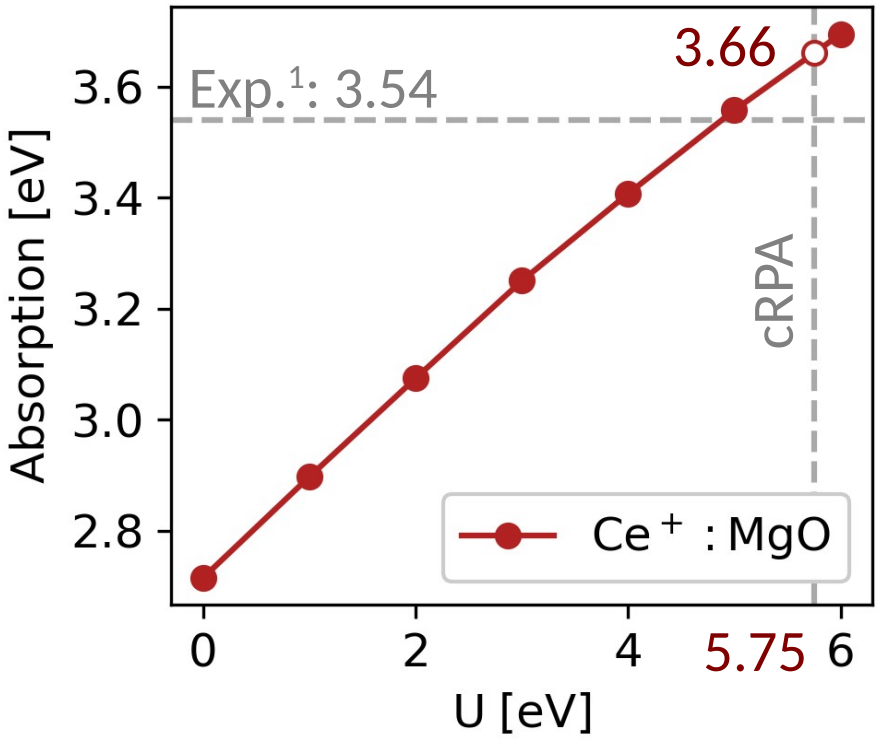
H. Ma et al., J. Chem. Theory Comput. **17**, 4, 2116 (2021).

Cerium Defect: Excitations and Matrix Elements



1 T. Kato, J. Lumin. **192**, 316 (2017).

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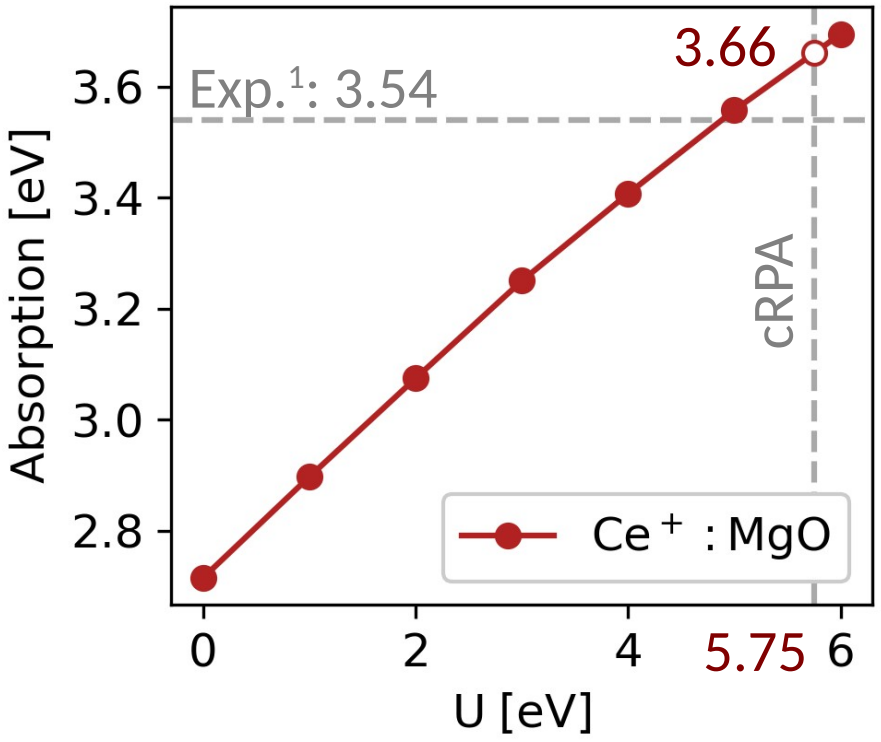

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THANK YOU FOR YOUR ATTENTION!