Exploring Exact Exchange

from an all-electron point of view

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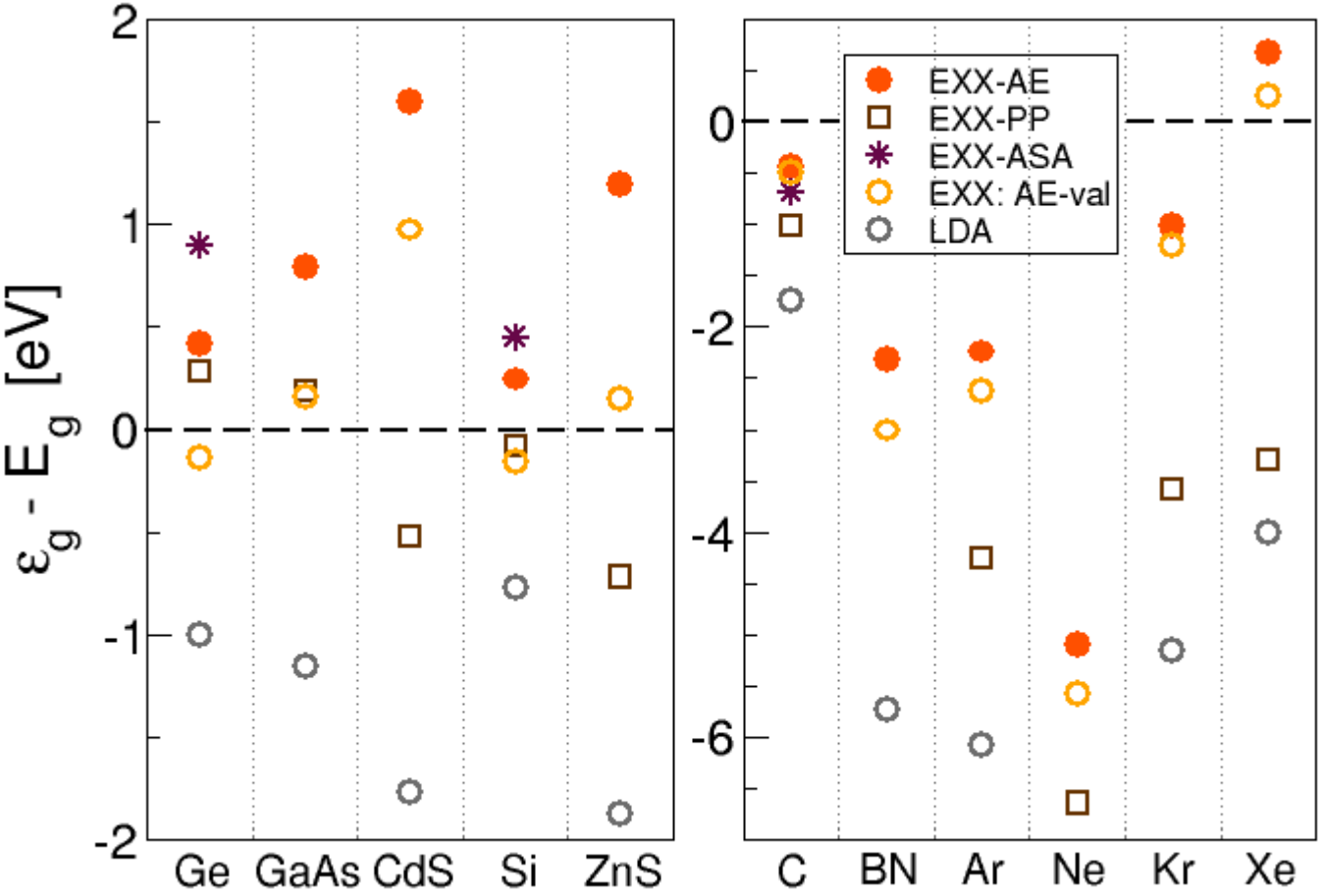
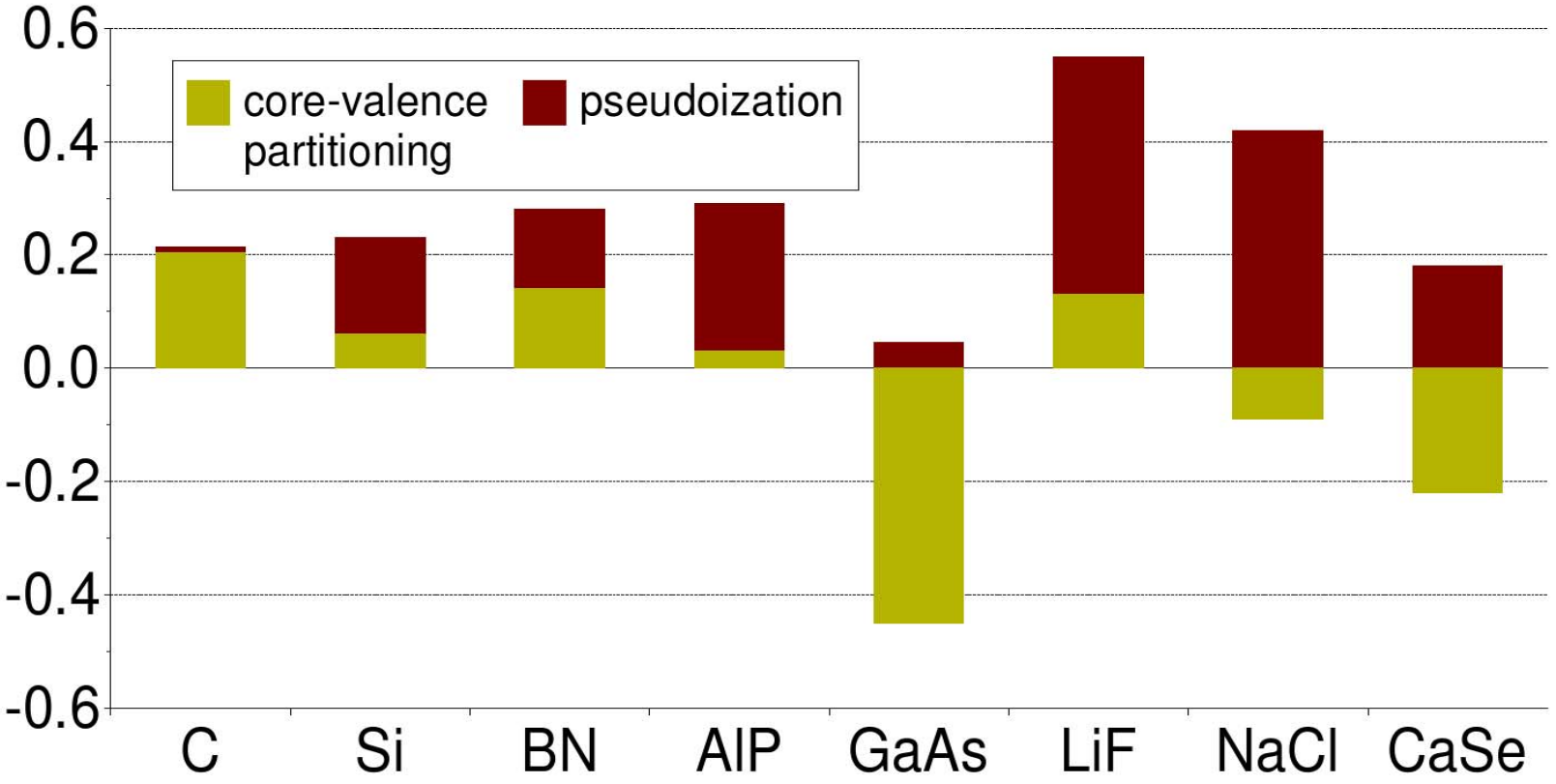
Band gaps



Städele et al., P. Rinke et al. , R. J. Magyar et al., T. Kotani
S. Sharma, J. K. Dewhurst, and CAD, Phys. Rev. Lett. 95, 136402 (2005)

All-electron versus PP G_0W_0

- PP errors due to two effects



R. Gómez-Abal, X. Li, M. Scheffler, and CAD, Phys. Rev. Lett. 101, 106404 (2008).

Support from GW

A closer look at G_0W_0

GaAs	ϵ^{KS}	Σ_c	Σ_x	V_{xc}	$\Sigma_x - V_{xc}$	ϵ^{qp}
All-electron G_0W_0:						
Γ_v	0.00	1.28	-16.85	-15.64	-1.21	0.00
Γ_c	0.25	-3.34	-12.22	-16.67	4.45	1.29
$\Gamma_c - \Gamma_v$ (Δ)	0.25	-4.62	4.63	-1.03	5.66	1.29
AE-valence G_0W_0 (Ga: 4s, 4p. As: 4s, 4p)						
Γ_v	0.00	1.00	-12.39	-11.38	-1.01	0.00
Γ_c	0.25	-3.17	-6.88	-10.63	3.75	0.84
$\Gamma_c - \Gamma_v$ (Δ)	0.25	-4.17	5.51	0.75	4.76	0.84
PP-G_0W_0						
Γ_v	0.00	0.82	-12.65	-11.24	-1.41	0.00
Γ_c	0.35	-3.29	-7.01	-10.33	3.32	0.97
$\Gamma_c - \Gamma_v$ (Δ)	0.35	-4.11	5.64	0.91	4.73	0.97

R. Gómez-Abal, X. Li, M. Scheffler, and CAD, preprint

Example: GaAs

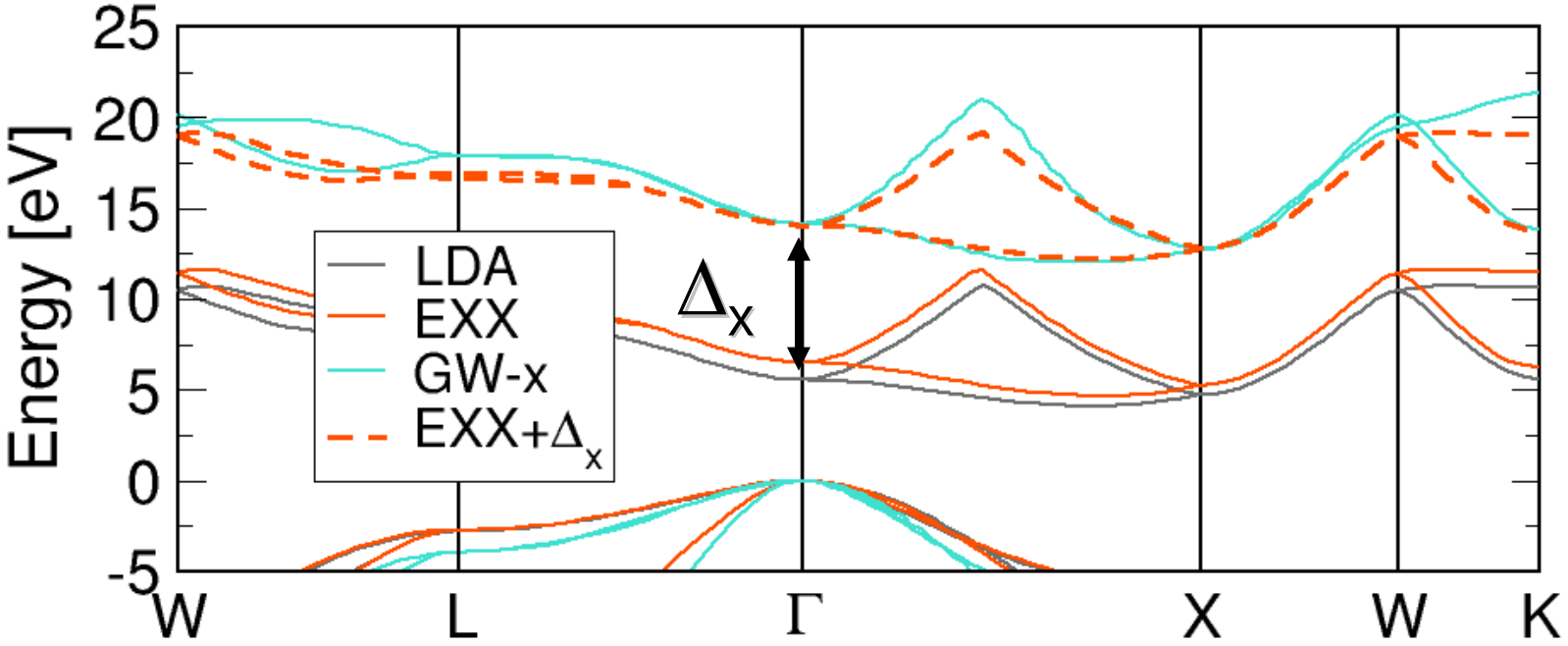
A closer look: G_0W_0 - x only

	ϵ_{LDA}	Σ^x	V^x	$\Sigma^x - V^x$	ϵ_{HF}
All-electron HF:					
Γ_v	0.00	-16.82	-14.02	-2.80	0.00
Γ_c	0.25	-12.14	-14.97	2.83	5.88
$\Gamma_v - \Gamma_v(\Delta)$	0.25	4.68	-0.95	5.63	5.88
AE-Valence HF ($4s$, $4p$):					
Γ_v	0.00	-12.30	-9.86	-2.56	0.00
Γ_c	0.25	-6.82	-9.17	2.35	5.04
$\Gamma_c - \Gamma_v(\Delta)$	0.25	5.48	0.69	4.79	5.04

Example: GaAs

EXX & GW-x

$$E_g = \varepsilon_g^{KS} + \Delta_x$$



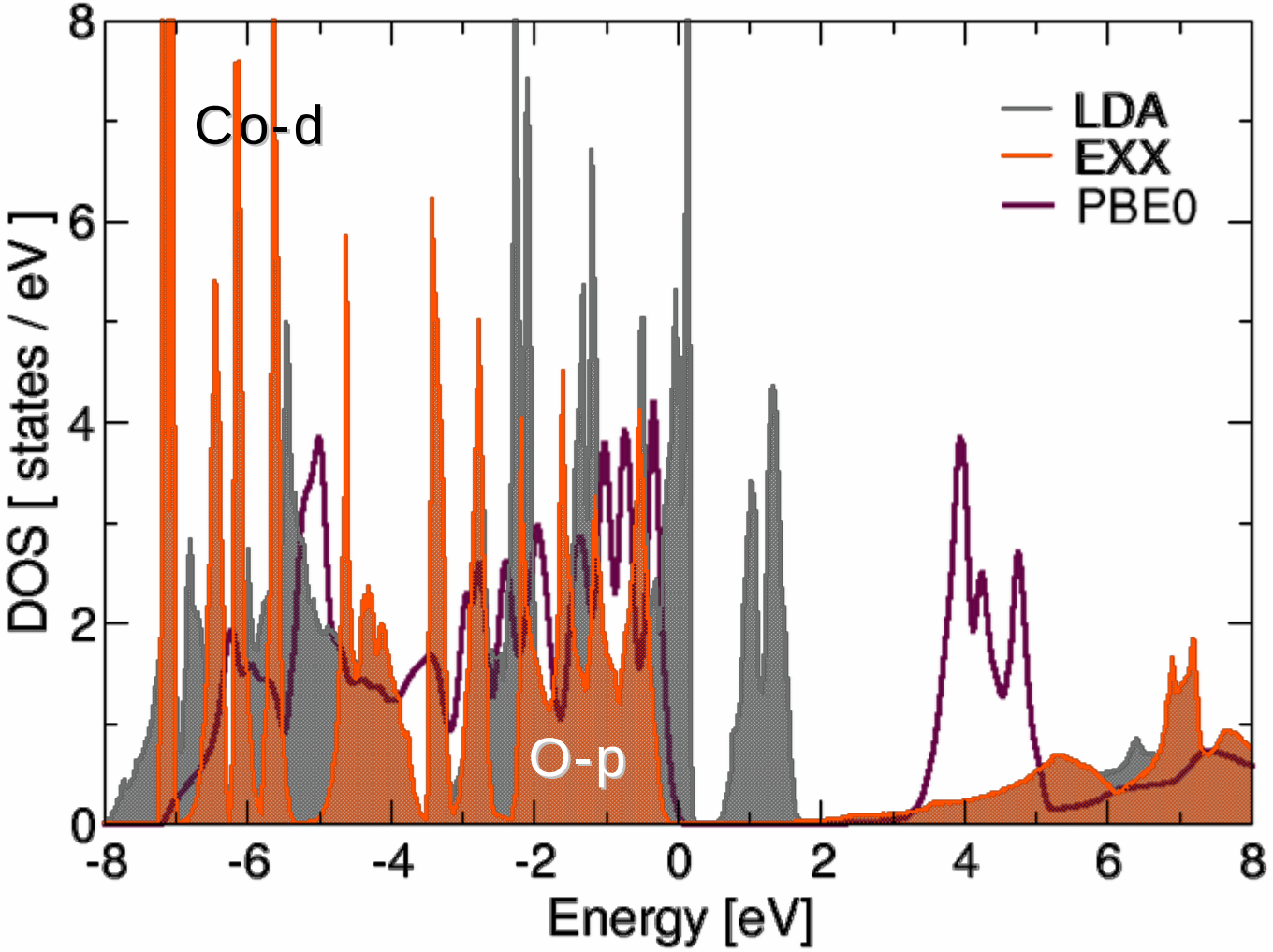
Example: Diamond

Magnetic moments [μ_B]

	Exp.	LSDA	EXX LAPW	EXX LMTO	HF / Hybrid
Fe	2.22	2.16	**2.6±0.1**	3.40	2.90
Co	1.71	1.62	**1.7±0.1**	2.25	1.90
Ni	0.56	0.70	**0.8±0.1**	0.68	0.76

LMTO: A. Kontani, J. Phys. Condens. Matter 10, 9421 (1998)
HF: I. Schnell, Phys. Rev. B 68, 245102 (2003)
Hybrid functionals: F. Tran et al., Phys. Rev. B 74, 155108 (2006)

Density of states



PBE0: F. Tran et al., Phys. Rev. B 74, 155108 (2006)

Example: CoO