CP2K PBE0 benchmarking for ionic crystals

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Materials considered NaCl, CsCl, AgCl, InCl3, Cs2InAgCl6.
PBC, Gamma point calculations. Target property: band gap.

CP2K 4.1 setups:

- All the primary basis sets are DZVP-MOLOPT-SR-GTH from BASIS_MOLOPT.
- All the ADMM basis sets are from BASIS_ADMM and BASIS_ADMM_MOLOPT.
- All the pseudopotentials are GTH-PBE from GTH_POTENTIALS with q9, q9, q13, q11, q7 for Na Cs, In, Ag, and Cl, respectively.
- CUTOFF=250 Ry, REL_CUTOFF=50 Ry.

VASP 5.4.4 setups:

- PAW potentials (recommended) with 7, 9, 13, 11, and 7 valence electrons for Na Cs, In, Ag, and Cl.
- PBE XC
- ENCUT=300 eV. (larger than the recommend ENMAX)

cp2k

	Natoms	PBE		PBE0			
		cp2k	vasp	adm_small	adm_large	vasp	Literature*
NaCl	216	4.93	4.99	7.04	7.03	7.09	7.13,7.26
InCl3	192	2.94	2.99	4.94	4.97	5.12	
AgCl	216	1.26	1.26	2.89	2.91	3.09	
CsCl	216	4.82	4.86	6.86	6.81	6.85	
CsInAgCl	320	1.14	1.15	2.65	2.63	3.23	3.3

	ADMM_SMALL	ADMM_LARGE
Cl	cFIT3	pFIT3
Na	cFIT3	pFIT3
Cs	cFIT7	FIT11
In	cFIT9	FIT13
Ag	cFIT9	FIT12

- *PRB 81, 195117,2010, JCP 124, 154709,2006
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- Note the finite size effect in the present calculations. Literature data were obtained using a converged k mesh.
- The Coulomb truncation was not used, since it represents the case with infinite R_c.

PBE0-TC-LRC of InCl3 →

R_c (A)	5	6	7	8	9	No_TC
Eg (eV)	4.916	4.931	4.935	4.939	4.940	4.943

Checking the CUTOFF/REL_CUTOFF for CP2K

InCl3	250/50	400/60
PBE	2.94	2.94
PBE0	4.94	4.94

CsInAgCl	250/50	400/60	600/60
PBE	1.14	1.13	1.13
PBE0	2.65	2.66	2.66