Supporting Information for Random phase approximation-based local natural orbital coupled cluster theory

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I. BASIS SETS AND GEOMETRIES

The solid-optimized cc-pVTZ basis sets for Cu, as well as the fitting basis sets for Cu and Li used in this work, are available in the following GitHub repository:

github.com/hongzhouye/supporting_data/tree/main/2026/RPALNOCC

The same repository also contains the structure files for the C2C2PD molecular dimer and the anthracene molecular crystal, including all geometries required for counterpoise corrections.

II. SUPPLEMENTARY DATA

TABLE S1. Lattice energy of the anthracene molecular crystal calculated by HF, MP2, and RPA using $1\times1\times1$ and $2\times2\times2$ k-point meshes and the cc-pVTZ basis sets. The thermodynamic limit (TDL) results are obtained by linearly extrapolating the two finite k-mesh results with N_k^{-1} to $N_k=\infty$.

N_k	HF	MP2		RPA	
		Correlation	Total	Correlation	Total
$1\times1\times1$	−75.4	−11.6	−86.9	−2.7	−78.0
$2\times2\times2$	+3.5	−46.2	−42.7	−25.5	−22.0
TDL	14.7	−51.1	−36.4	−28.8	−14.0

TABLE S2. Per-atom correlation energy calculated by different methods for BCC Li and FCC Cu using different basis sets and k-point meshes. The CCSD results for $2\times2\times2$/DZ and $3\times3\times3$/DZ are from canonical k-point CCSD, while all others are the best extrapolated values from LNO-CCSD as explained in the main text.

System	N_k	Basis set	MP2	RPA	RPA+SOSEX	CCSD
BCC Li	$3\times3\times3$	TZ	-0.0604	-0.0862	-0.0488	-0.0630
	$2\times2\times2$	DZ	-0.0344	-0.0478	-0.0276	-0.0388
BCC Li	$3\times3\times3$	DZ	-0.0463	-0.0535	-0.0325	-0.0434
	$4\times4\times4$	DZ	-0.0534	-0.0557	-0.0346	-0.0452
FCC Cu	$2\times2\times2$	TZ	-0.5583	-0.4823	-0.3789	-0.4690