Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Energy level modeling of lanthanide materials: review and uncertainty analysis

Electronic supplementary information

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S1 Illustrative cartoon

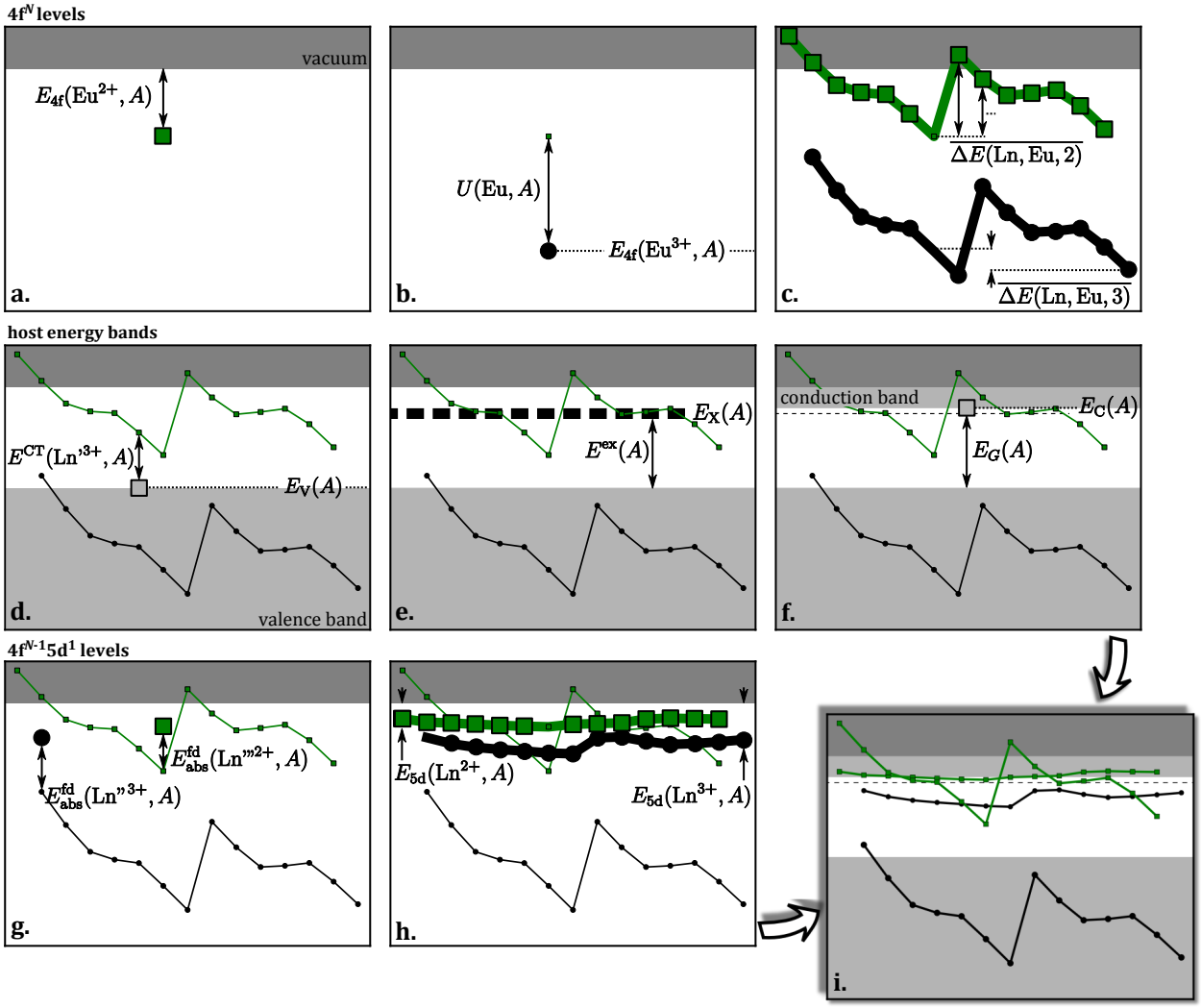

Figure S1 Illustrative cartoon on how to obtain an energy level scheme from the calculated quantities.

S2 Table of $4f^N$-$4f^{N-1}6s^1$ transition energies

Table S1 The energy of the lowest $4f^N$-$4f^{N-1}6s^1$ transition in free Ln^{3+} and Ln^{2+} ions. If the spectroscopic redshift, $D^{\mathrm{fs}}(Q,A)$, of the electronic transition is known for one Ln^{Q+} in host A, the same reasoning as for the $4f^{N-1}5d^1$ manifold is expected to hold and $4f^{N-1}6s^1$ energy levels can be added to the energy level schemes. Collected from [1–17]. If no experimental energy was available, the estimate from [11] was adopted. All values in eV.

Ln	$E^{\mathrm{fs}}(Ln^{2+},\mathrm{free})$	$E^{\mathrm{fs}}(Ln^{3+},\mathrm{free})$
La	0.79	
Ce	2.39	10.74
Pr	3.52	12.43
Nd	3.76	13.65
Pm	3.65	13.76
Sm	4.49	13.66
Eu	5.95	14.53
Gd	0.84	15.55
Tb	2.19	10.92
Dy	2.86	12.29
Ho	2.71	12.98
Er	2.40	12.84
Tm	3.14	12.27
Yb	4.30	13.14
Lu		14.48

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