Computational studies of material properties in $CuInSe_2$ photovoltaic solar cell material

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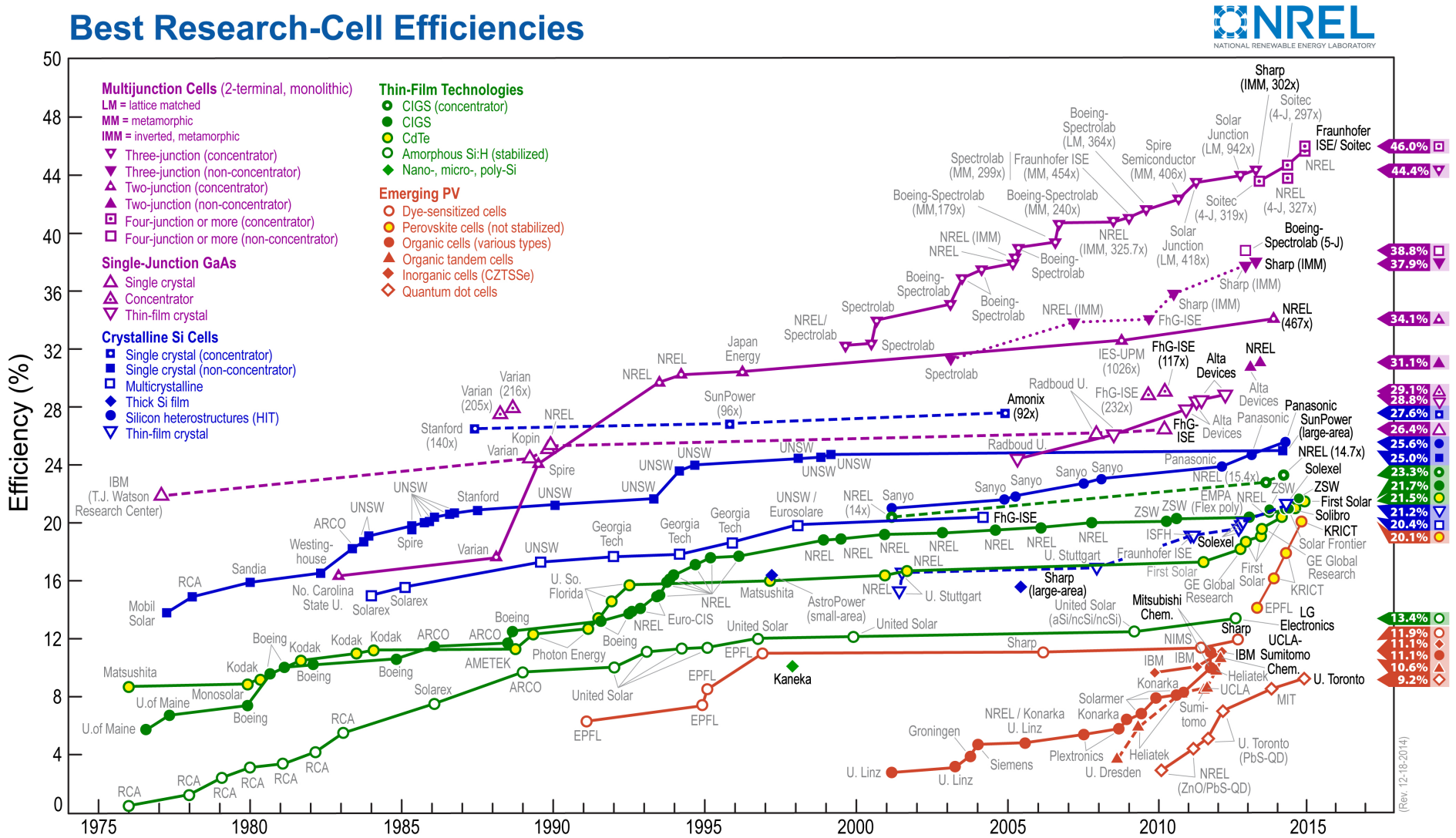
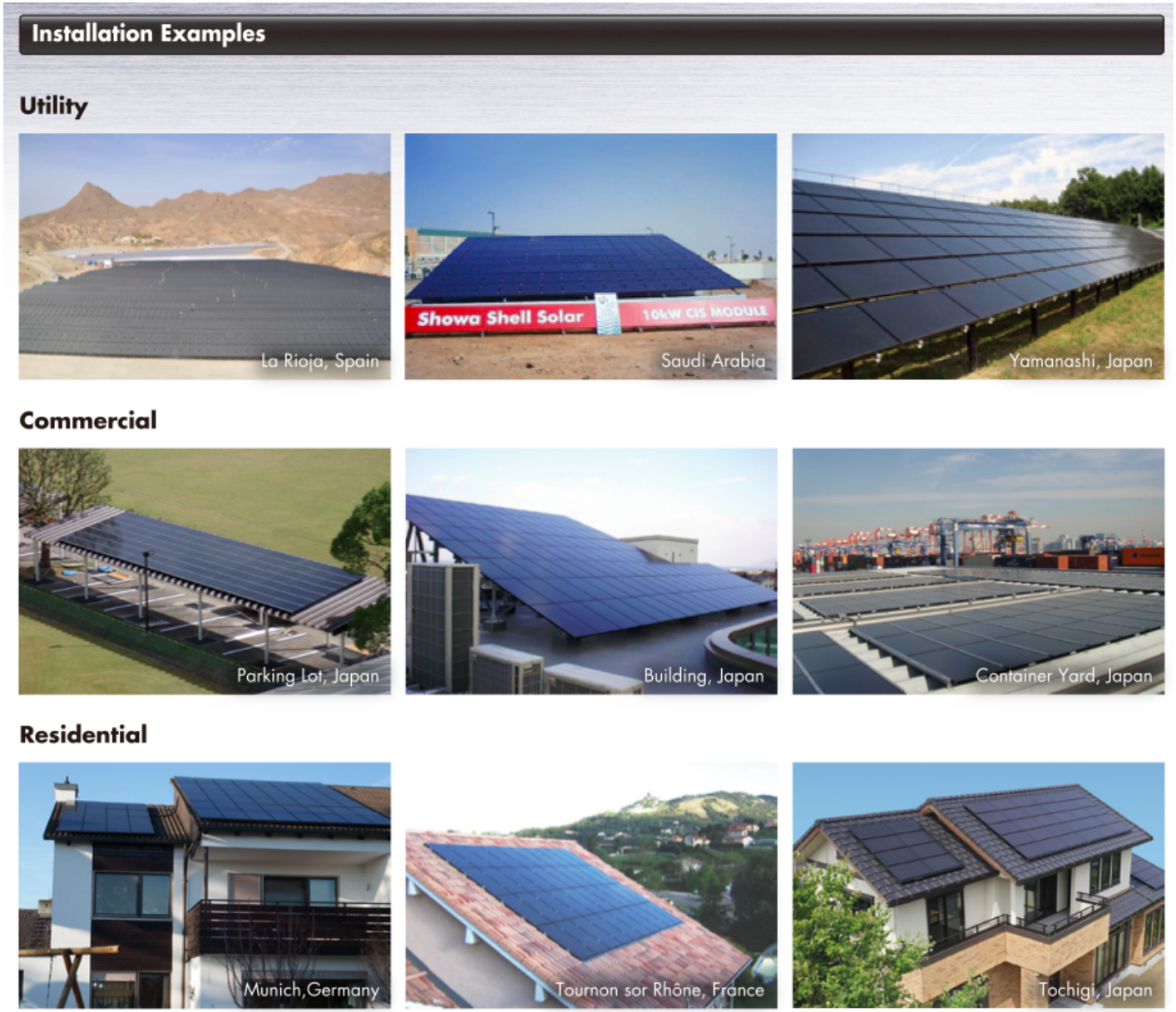
Outline


Best Research-Cell Efficiencies
NREL
NATIONAL RENEWABLE ENERGY LABORATORY
Efficiency (%)
Multijunction Cells (2-terminal, monolithic)
LM = lattice matched
MM = metamorphic
IMM = inverted, metamorphic
Three-junction (concentrator)
Three-junction (non-concentrator)
Two-junction (concentrator)
Two-junction (non-concentrator)
Four-junction or more (concentrator)
Four-junction or more (non-concentrator)
Single-Junction GaAs
Single crystal
Concentrator
Thin-film crystal
Crystalline Si Cells
Single crystal (concentrator)
Single crystal (non-concentrator)
Multicrystalline
Thick Si film
Silicon heterostructures (HIT)
Thin-film crystal
Thin-Film Technologies
CIGS (concentrator)
CIGS
CdTe
Amorphous Si:H (stabilized)
Nano-, micro-, poly-Si
Emerging PV
Dye-sensitized cells
Perovskite cells (not stabilized)
Organic cells (various types)
Organic tandem cells
Inorganic cells (CZTSSe)
Quantum dot cells
46.0%
44.4%
38.8%
37.9%
34.1%
31.1%
29.1%
28.8%
27.6%
26.4%
25.6%
25.0%
23.3%
21.7%
21.5%
21.2%
20.4%
20.1%
13.4%
11.9%
11.1%
11.1%
10.6%
9.2%
(Rev. 12-18-2014)

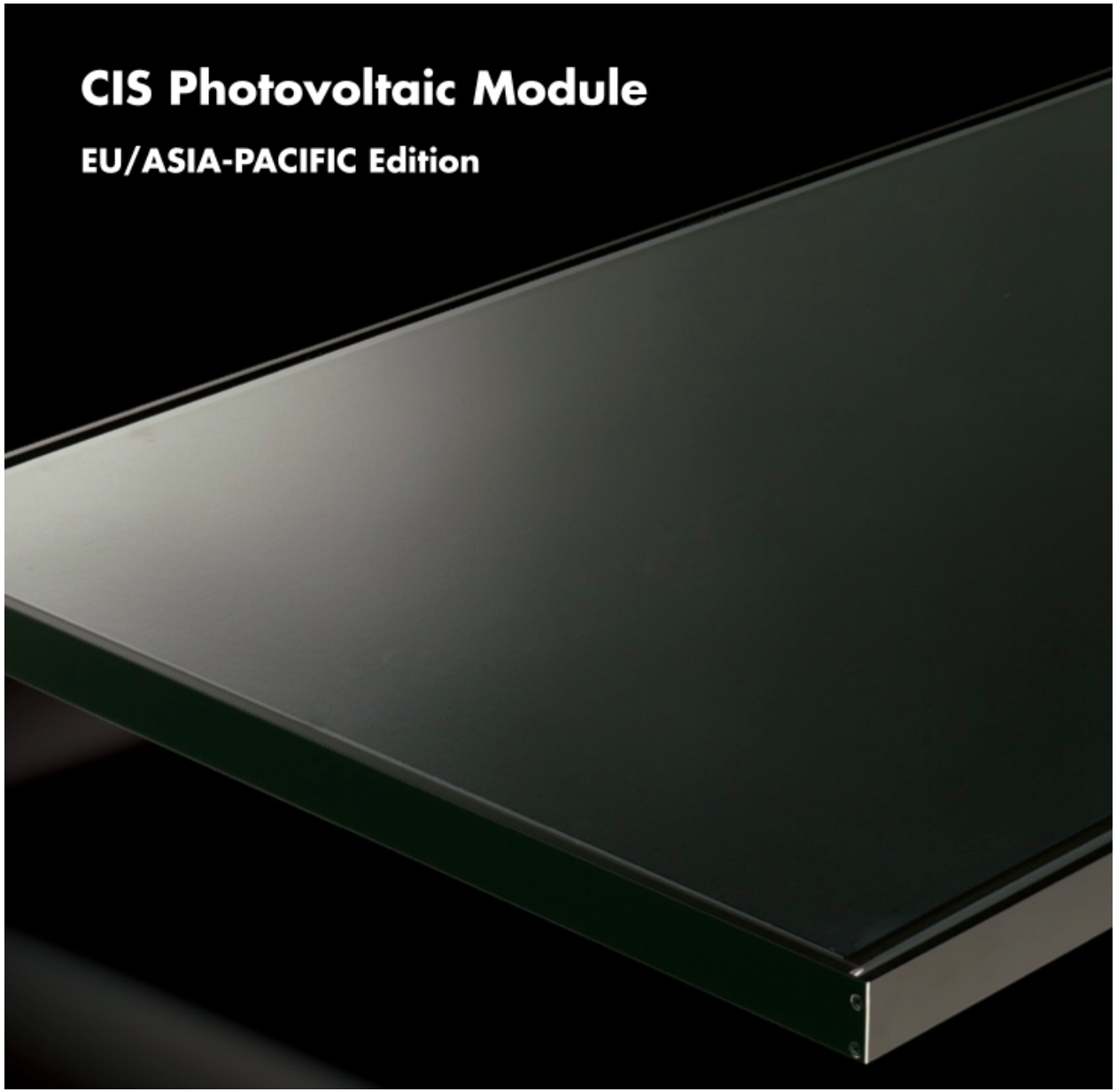
CIGS

- Material with direct band gap used in thin-film solar cells
- Used in photo-voltaics: Generation of electron-hole pairs that are separated and collected
- High efficiency, $>$ 20% demonstrated
- Band gap can be tuned from 1.0 (CIS) to 1.7 eV (CGS)

CIGS: Commercialisation



CIGS: Commercialisation



CIGS: Commercialisation

Company Profile

Headquartered in Tokyo, Japan, Solar Frontier is committed to the superior potential of CIS technology to set the world's standard for converting sunlight into usable energy. Based on more than 30 years of research and development, we are committed to leading the world in developing the full potential of CIS with an investment now exceeding $1 billion. This makes Solar Frontier the world's largest manufacturer of CIS solar panels, at more than 1GW of annual production capacity, primarily at our 1GW plant in Miyazaki, Japan.

SOLAR FRONTIER

Solar Frontier

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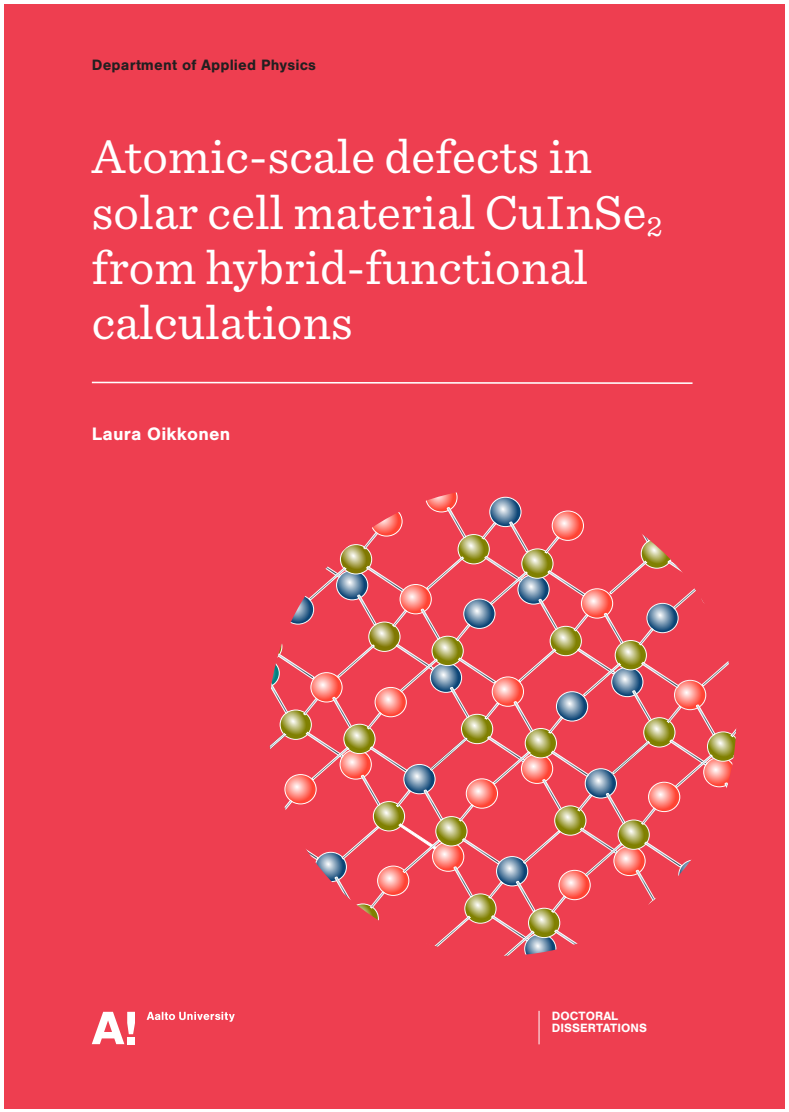
E-mail:info@solarfrontier.co.jp

CIGS: Computational modelling of defects

- Defects always present; affect properties of host material
- Point defects: Vacancies, inter-stitials, anti-sites
- Impurities, grain boundaries, . . .
- Our goal: Modelling of point defects and Na impurity in order to support and understand experimental results
- Density functional theory calculations

CIS: PhD thesis of Laura Oikkonen

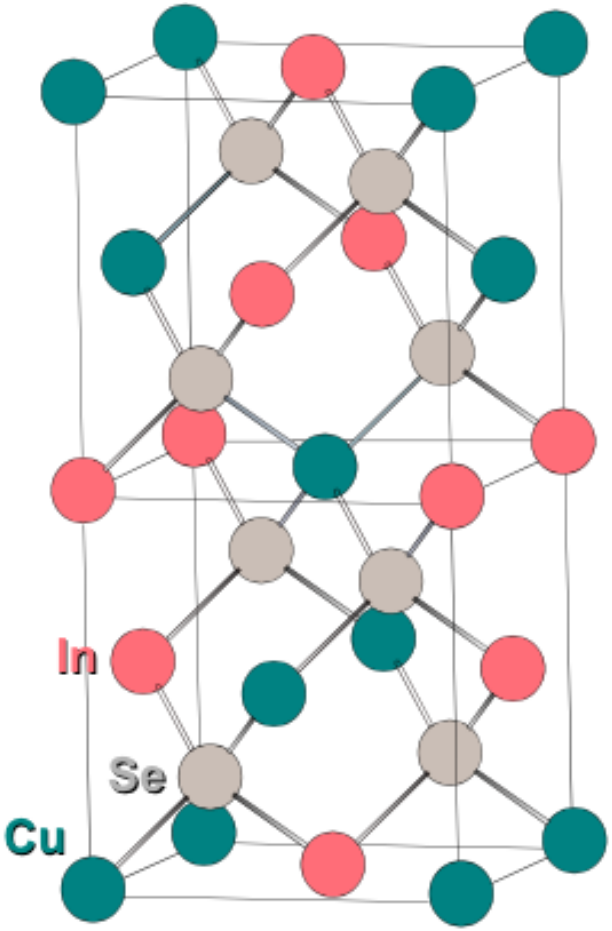


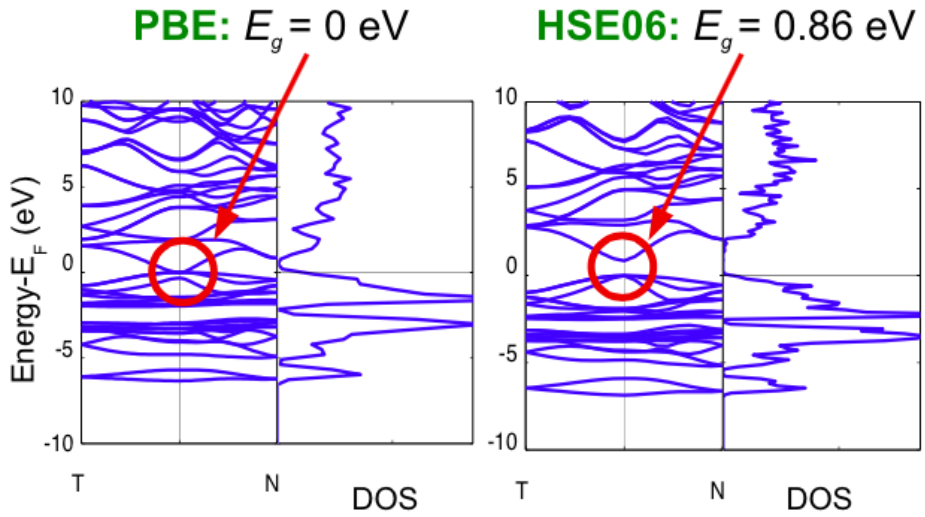
Laura E Oikkonen, Maria G Ganchenkova, Ari P Seitsonen, Rirsto M Nieminen

- I Vacancies in $CuInSe_2$: New insights from hybrid-functional calculations. Journal of Physics: Condensed Matter, 23, 422202, October 2011
- II Redirecting focus in $CuInSe_2$ defect studies towards selenium-related defects. Physical Review B, 86, 165115, October 2012
- III Mass transport in $CuInSe_2$ from first principles. Journal of Applied Physics, 113, 133510, April 2013
- IV Formation, migration, and clustering of point defects in $CuInSe_2$ from first principles. Submitted to Physical Review B, May 2013
- V Effect of sodium incorporation into $CuInSe_2$ from first principles. Journal of Applied Physics, 114, 083503, August 2013
- VI Formation, migration and clustering of point defects in $CuInSe_2$ from first principles. Journal of Physics: Condensed Matter, 26, 34, 345501, August 2014

Outline

Method: Density Functional Theory

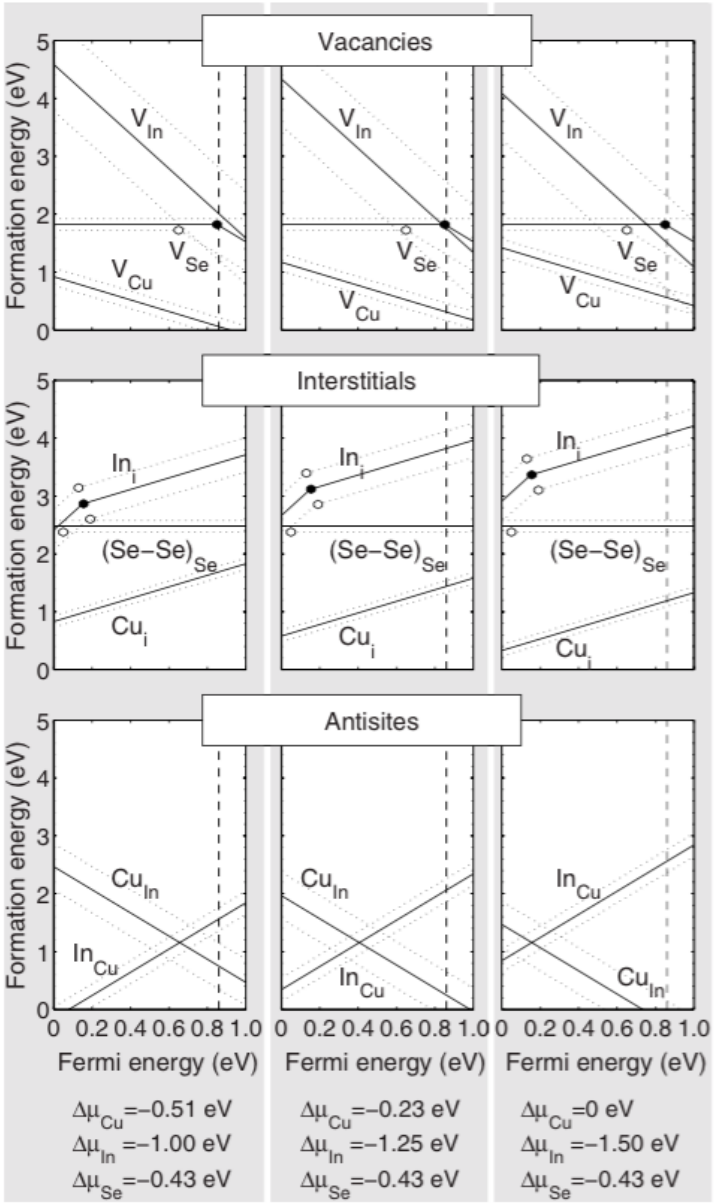




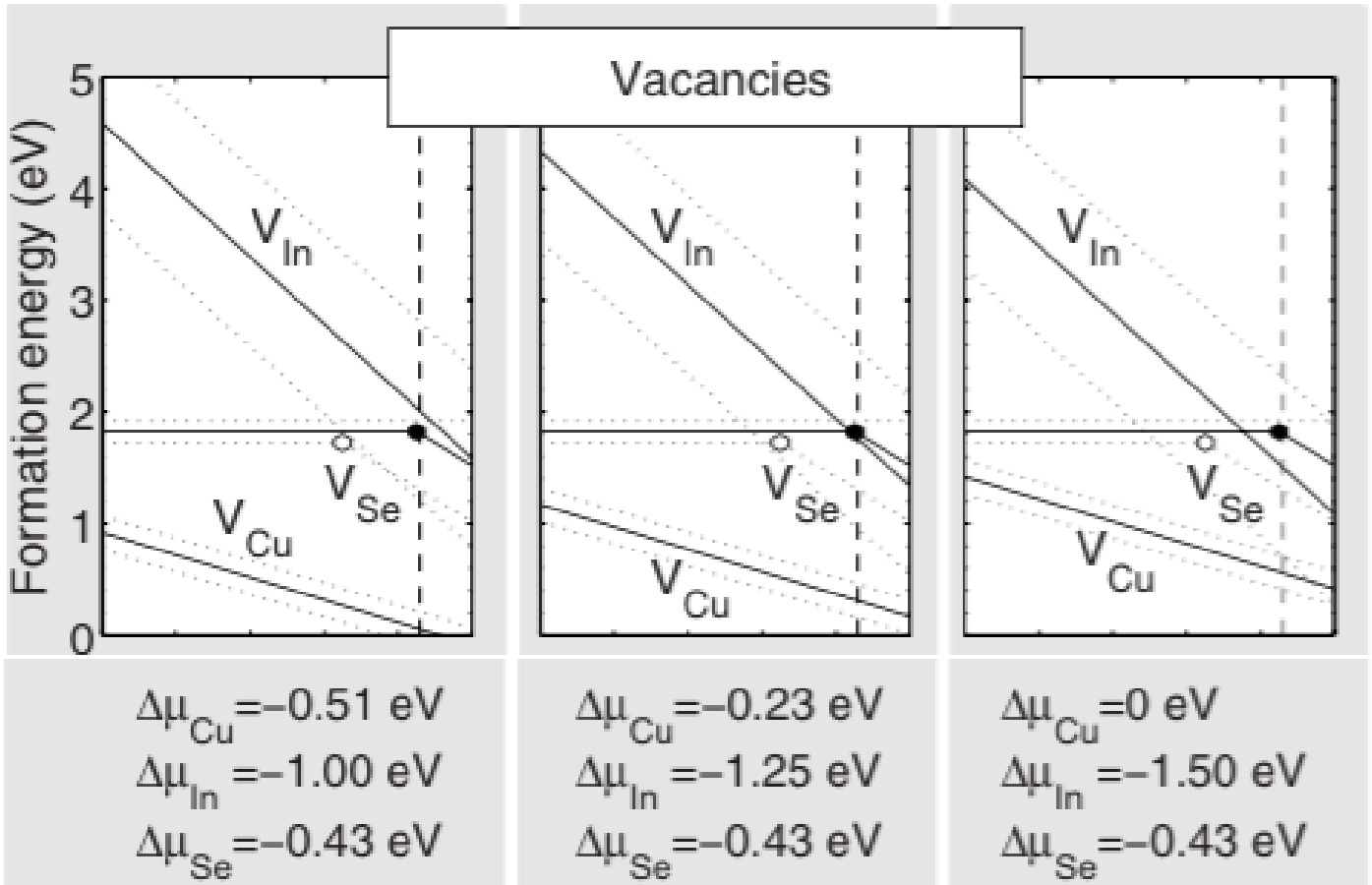
- DFT-hybrid functionals (HSE06)
- Supercells with 32-144 atoms (GGA up to 512)
- Finite-size scaling

Outline

CIS: Formation energy of defects



CIS: Formation energy of vacancies

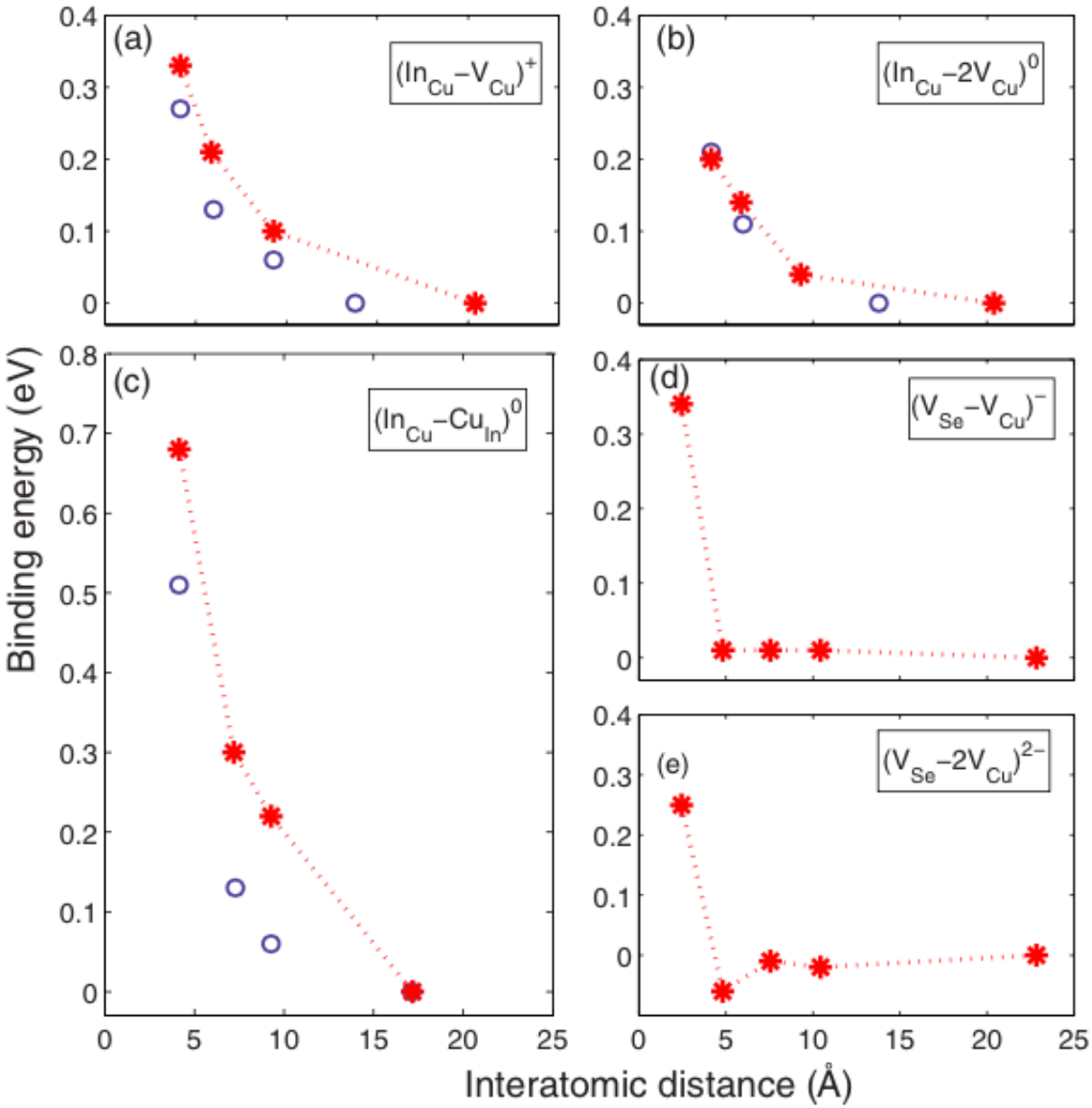


Formation energies depend on chemical potential of

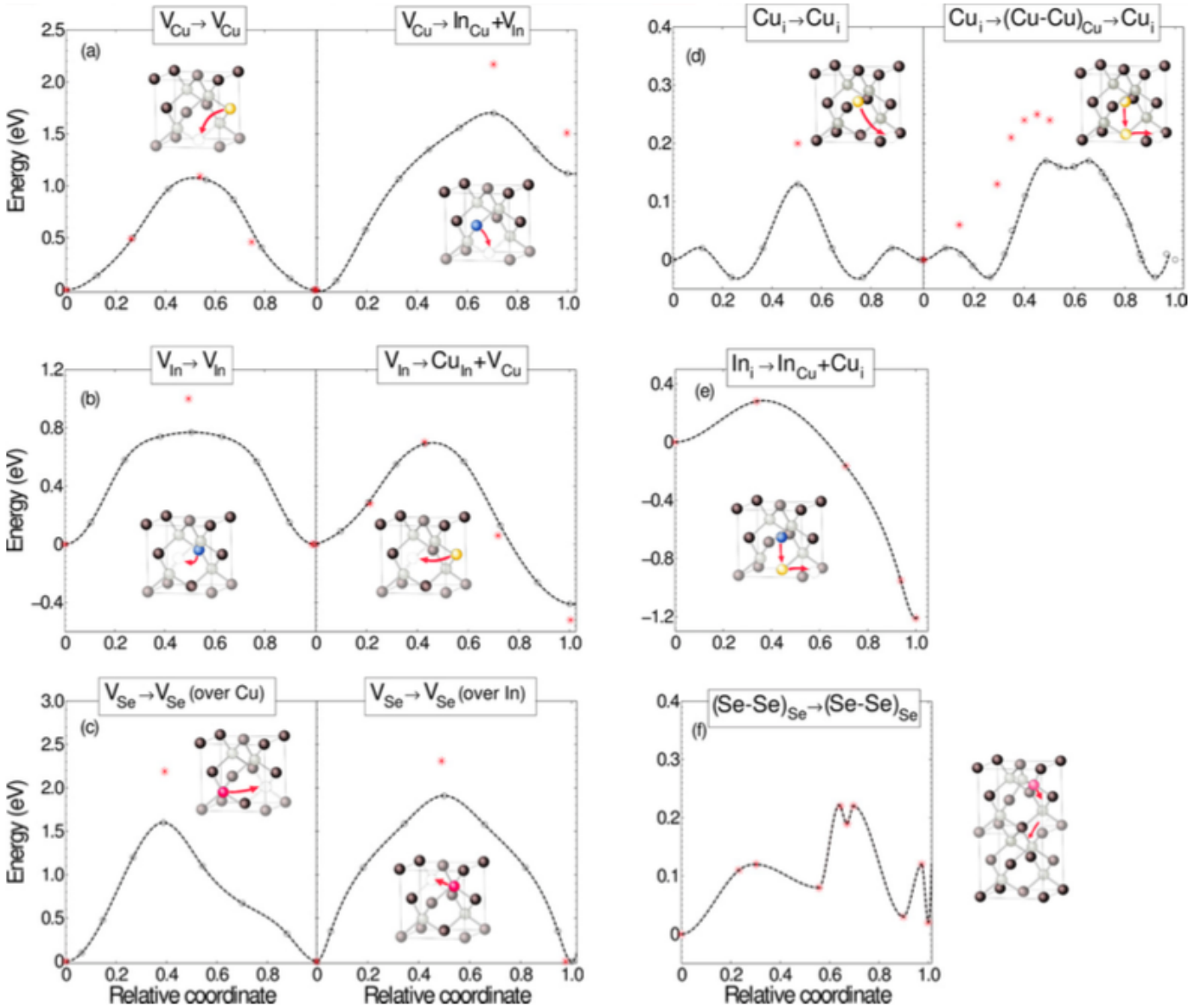
- electrons and ions

id est preparation conditions of sample

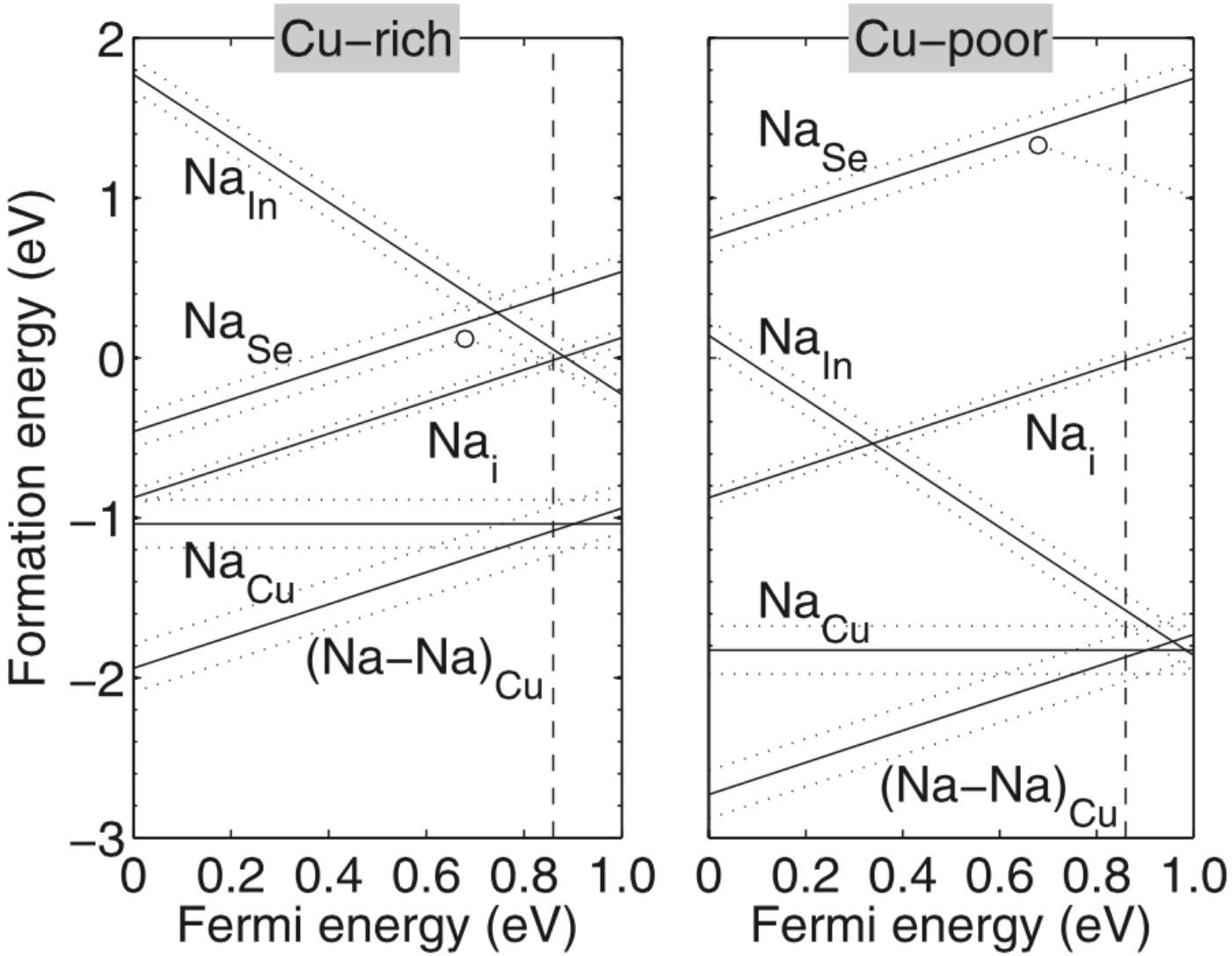
CIS: Binding/interaction energy of defects



CIS: Migration of defects



CIS+Na: Formation energy of defects

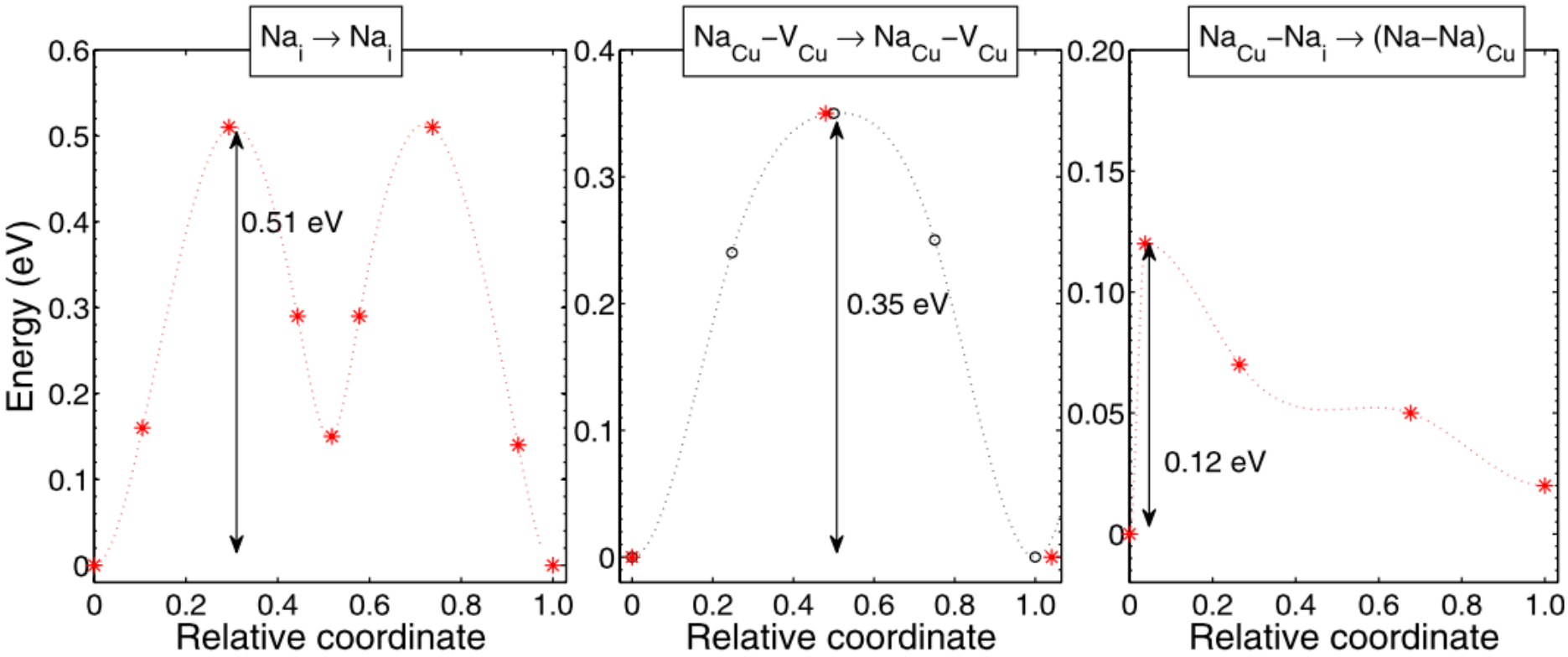


CIS+Na: Binding/interaction energy of defects

TABLE I. Binding energies (E_b) of Na-related defect complexes. The charge states of the isolated defects are 1– for V_{Cu}, 0 for Na_{Cu}, and 1+ for Na_i.

Complex	Charge state	E_b (eV)
$Na_{Cu} - V_{Cu}$	1–	0.00
$Na_{Cu} - 2V_{Cu}$	2–	–0.05
$2Na_{Cu}$	0	–0.03
Na_{Cu}–Na_i	1+	0.12
$(Na - Na)_{Cu}$	1+	0.12
$2(Na - Na)_{Cu}$	2+	0.15

CIS+Na: Migration of defects

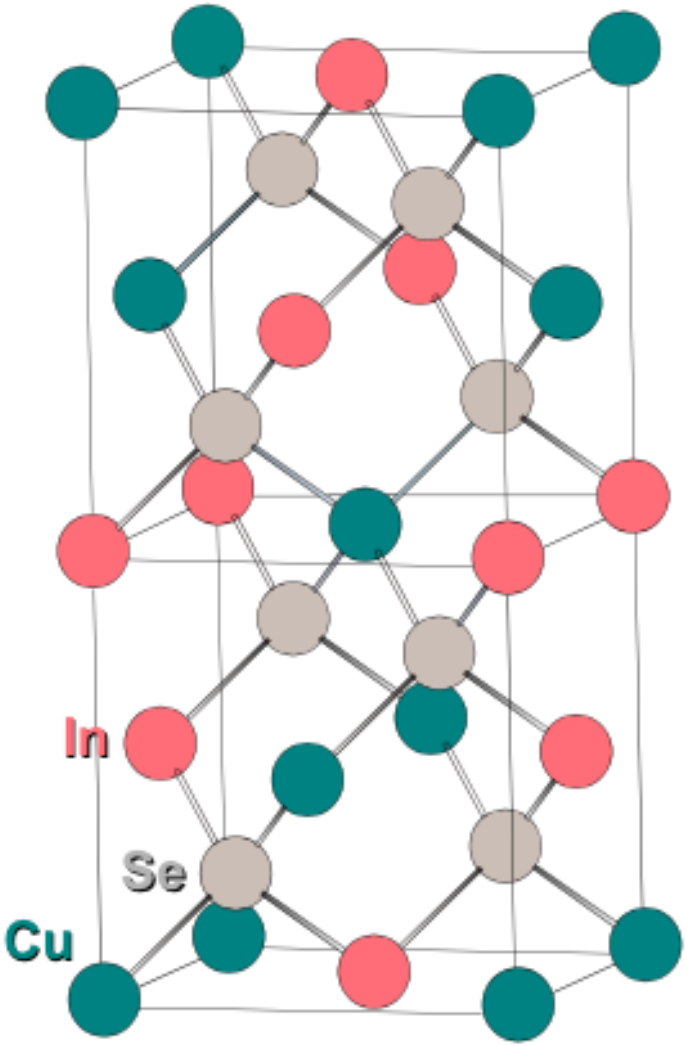


Barrier for $\mathrm{Na_{Cu}} - V_{\mathrm{Cu}} \leftrightarrow V_{\mathrm{Cu}} - \mathrm{Na_{Cu}}$ lower than for diffusion of V_{Cu}

$\Rightarrow$ Trapping of Cu vacancies by Na

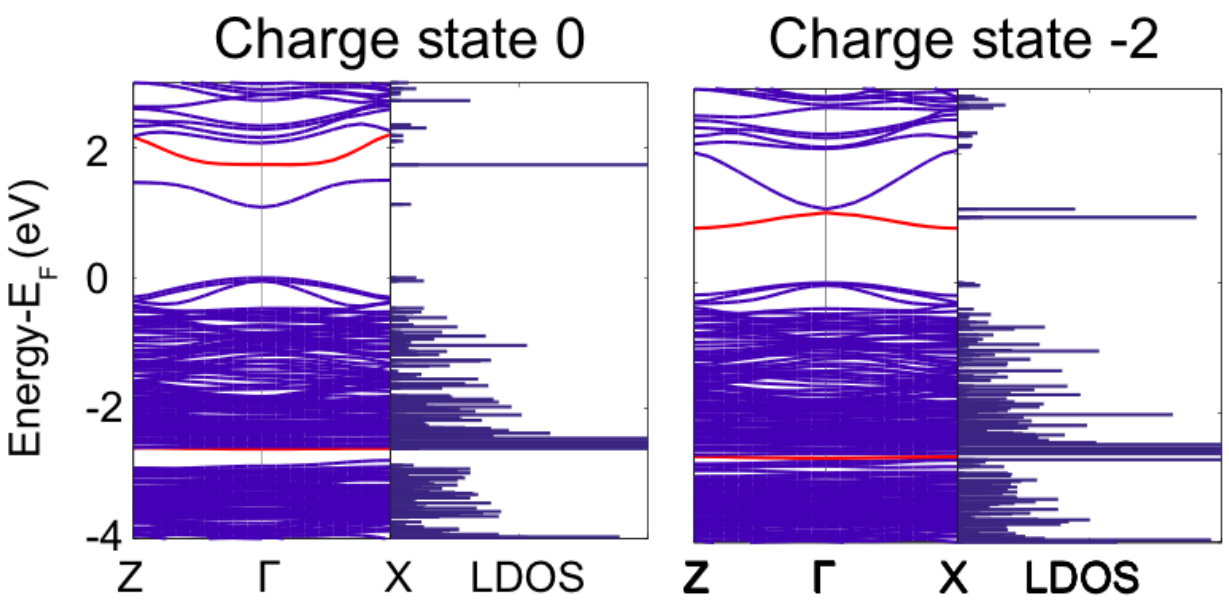
Outline

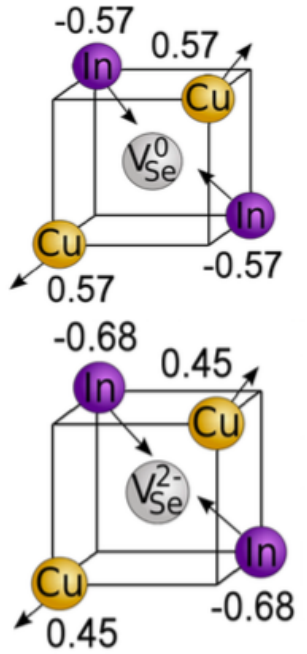
Summary



- DFT-hybrid functional calculations
- Point defects: Se-related defects most relevant due to states in gap
- Clustering, migration of defects investigated
- Na impurity traps Cu vacancies
- Things not shown (because not yet done): Grain boundaries, electric fields, interfaces, ...

CIS: Selenium vacancy

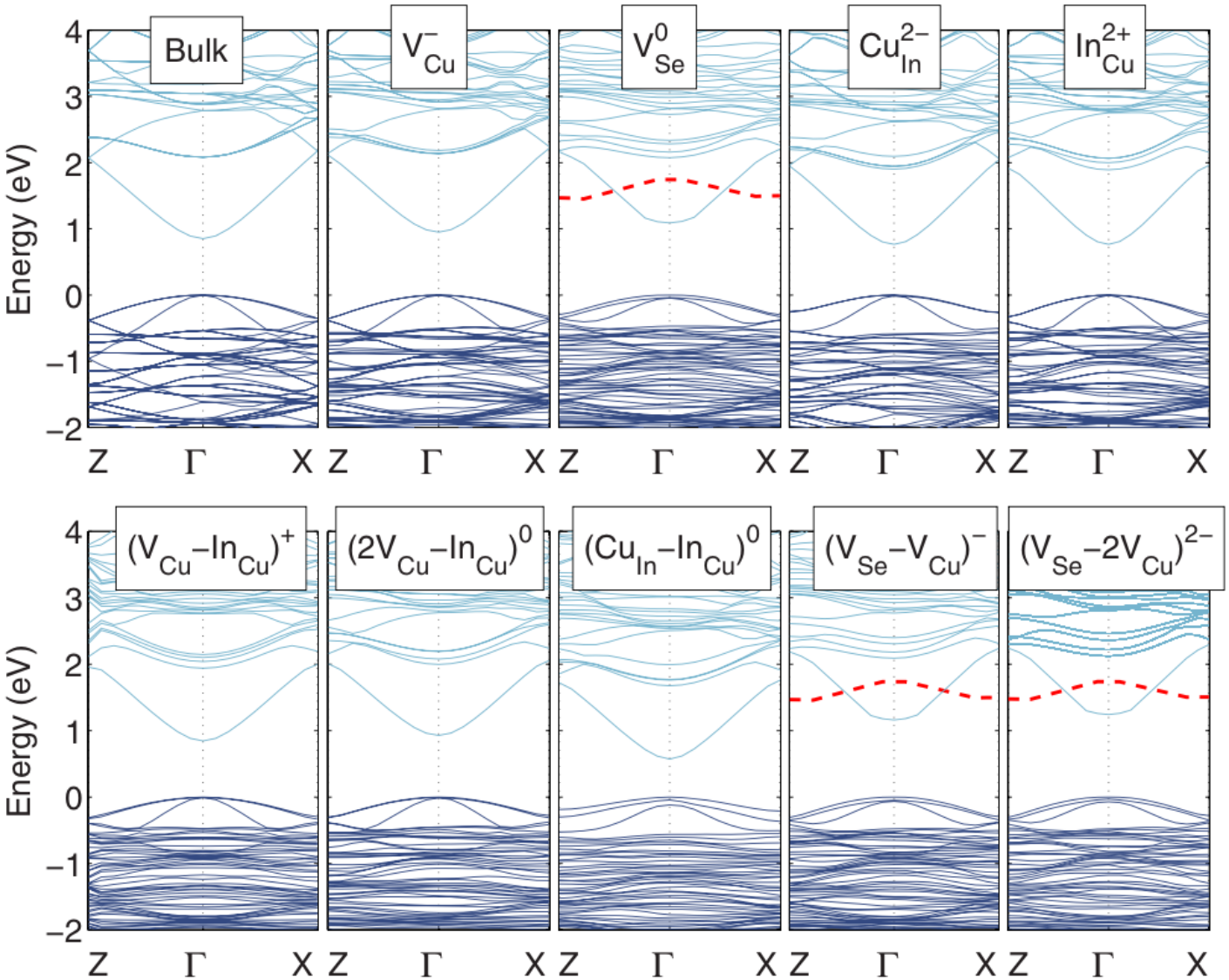




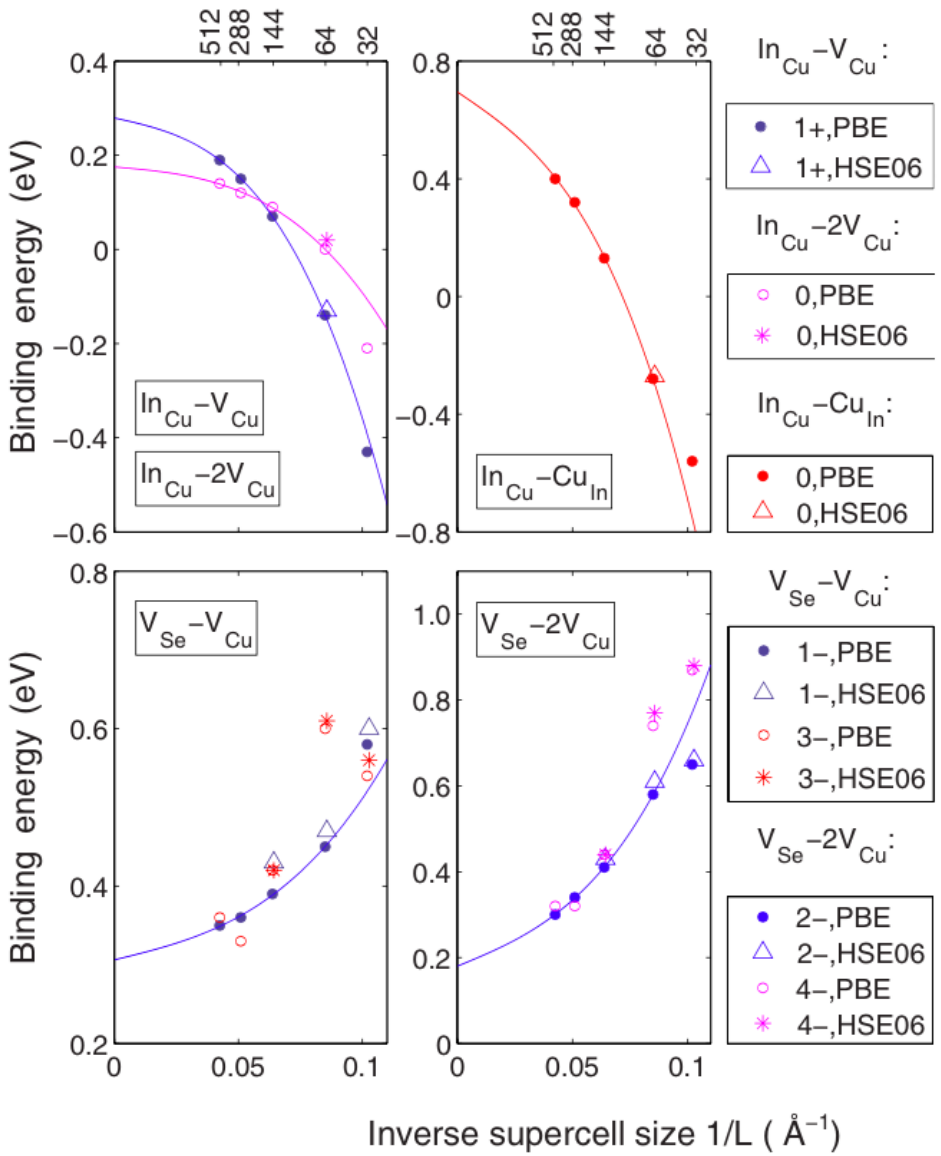
Atomic displacements expressed in Å

- Two stable charge states: 0 and -2
- Ionization level $\varepsilon(0/-2) = E_{VBM}+0.85$ eV

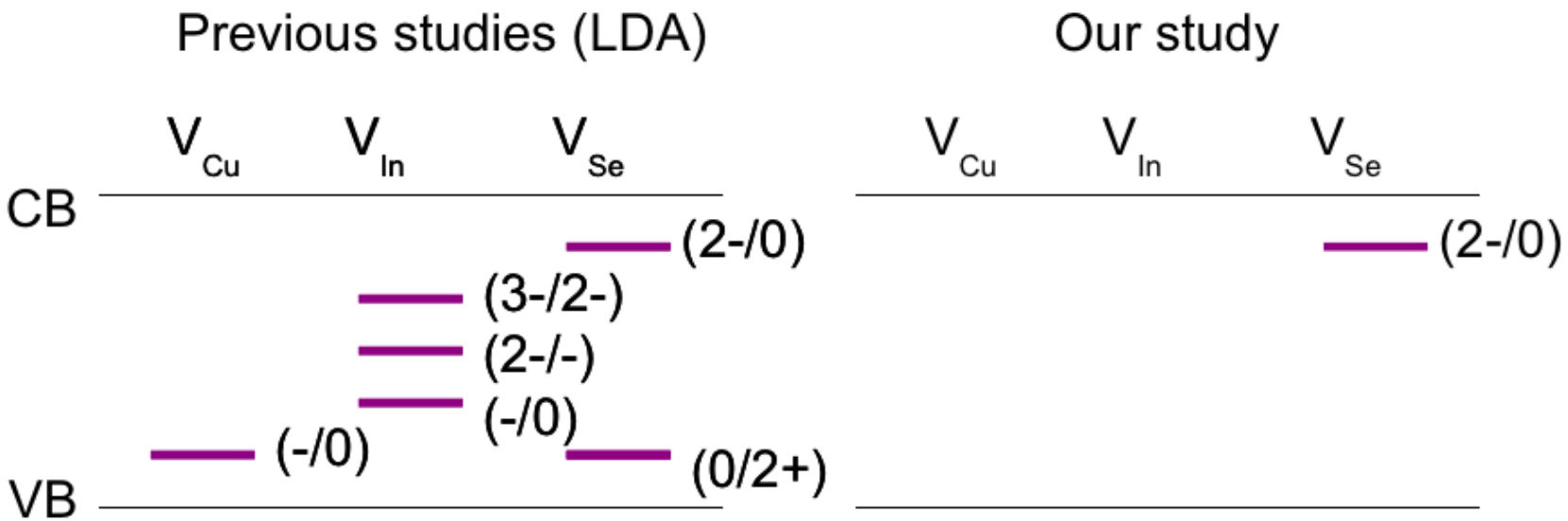
CIS: Band structures



CIS: Finite-size scaling



CIS: Comparison of defect formation energies



CIS+Na: Band structures