Atomistic Origins of Charge Traps in CdSe nanoclusters

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SUPPORTING INFORMATION

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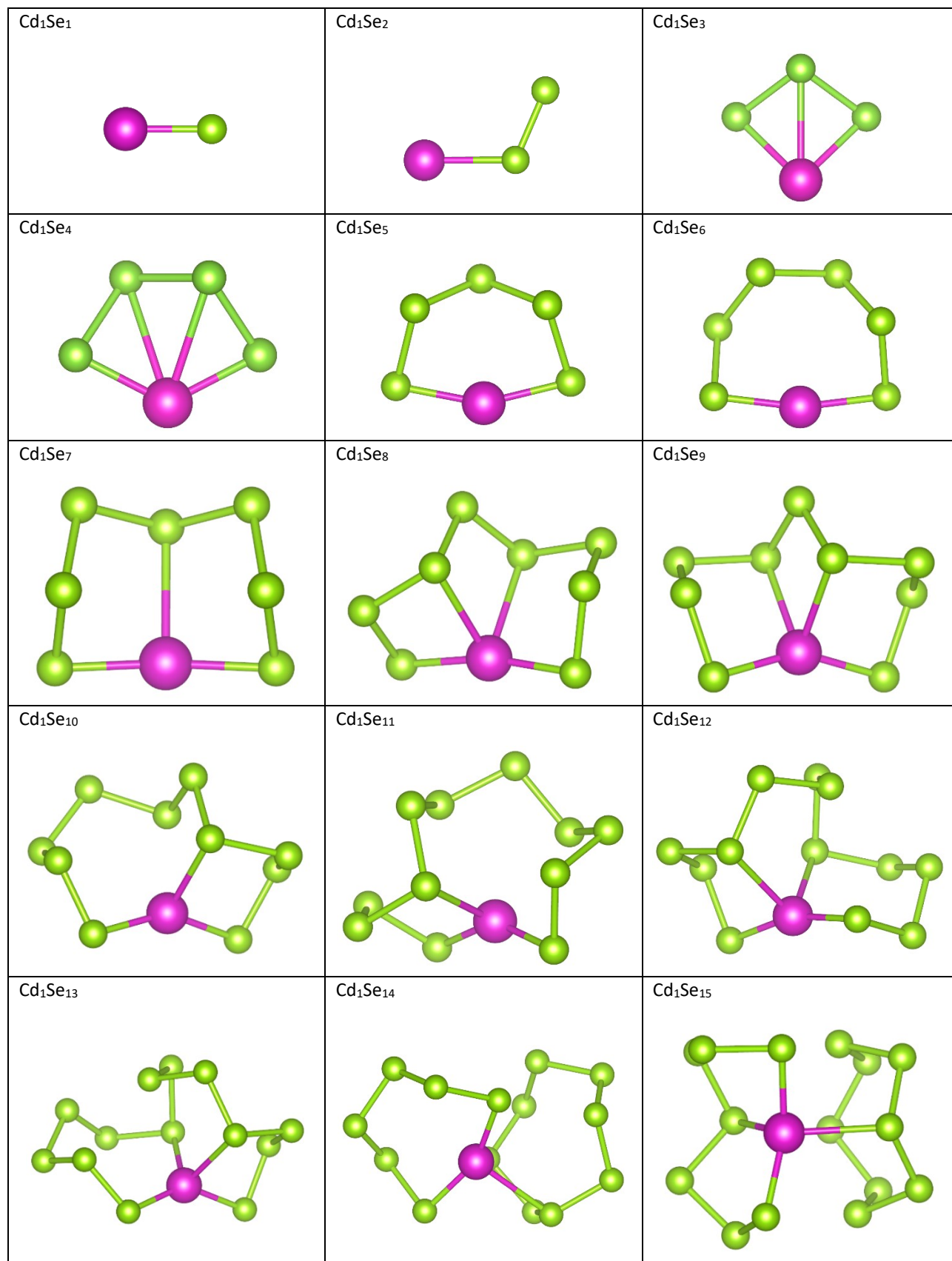
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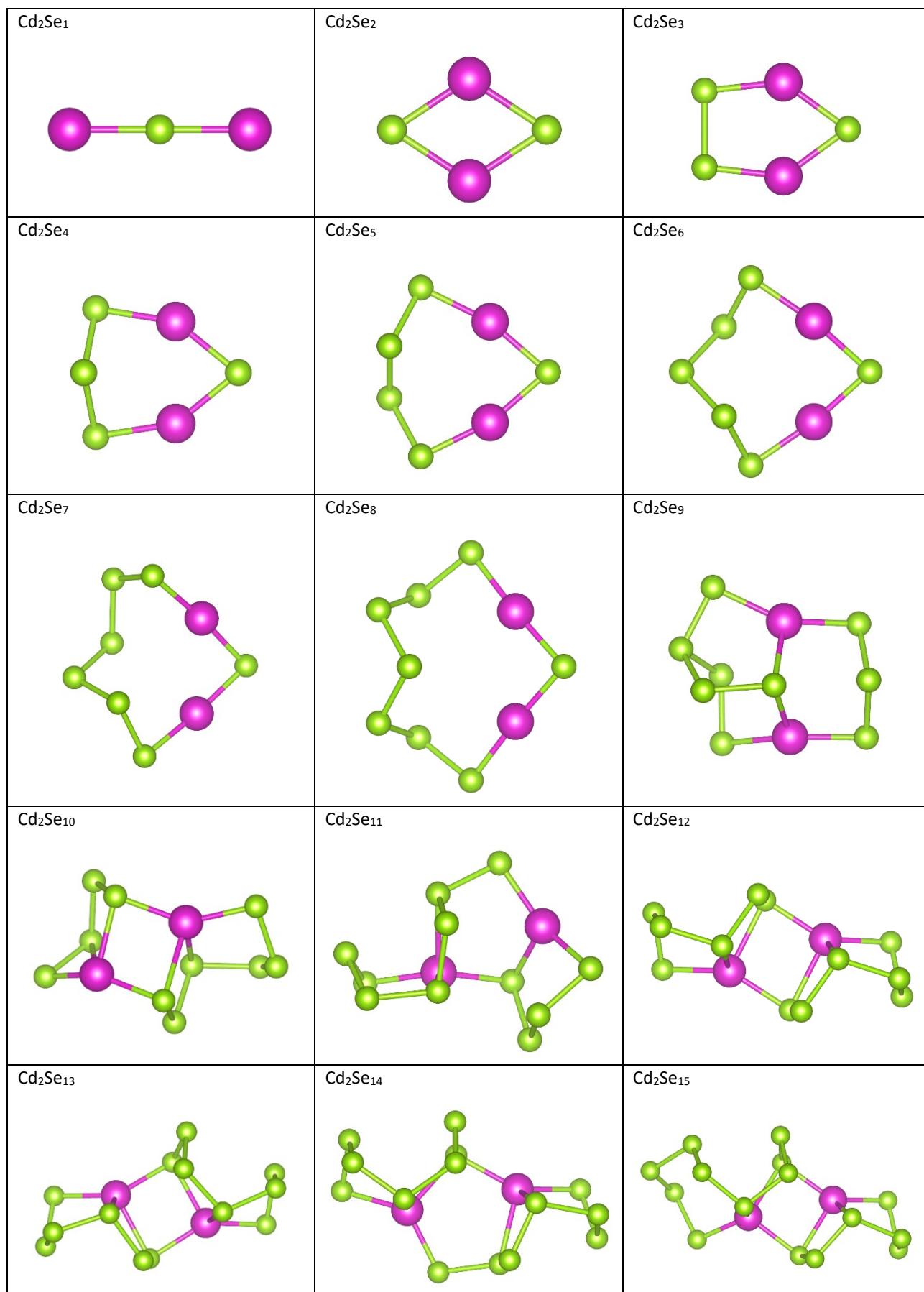
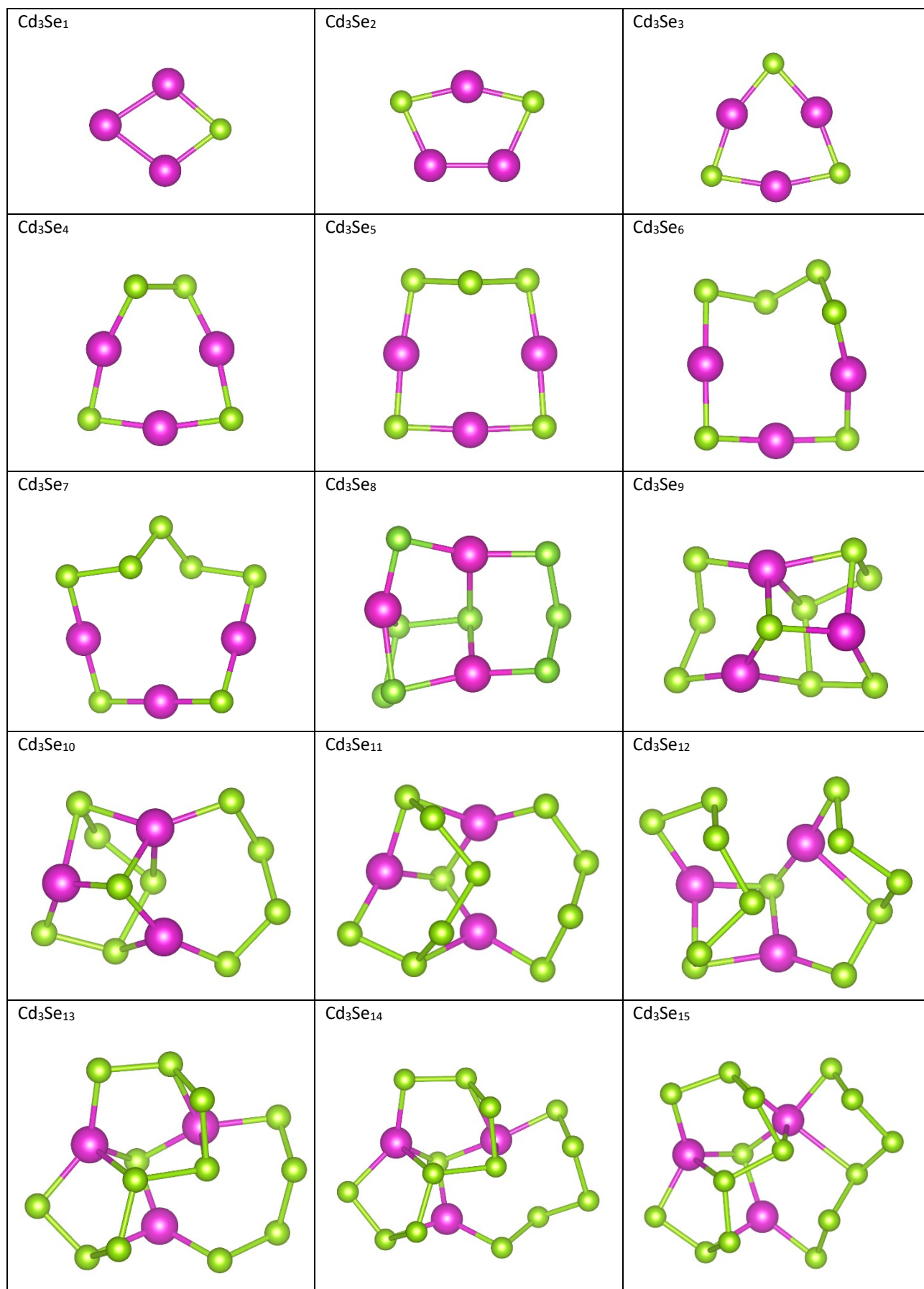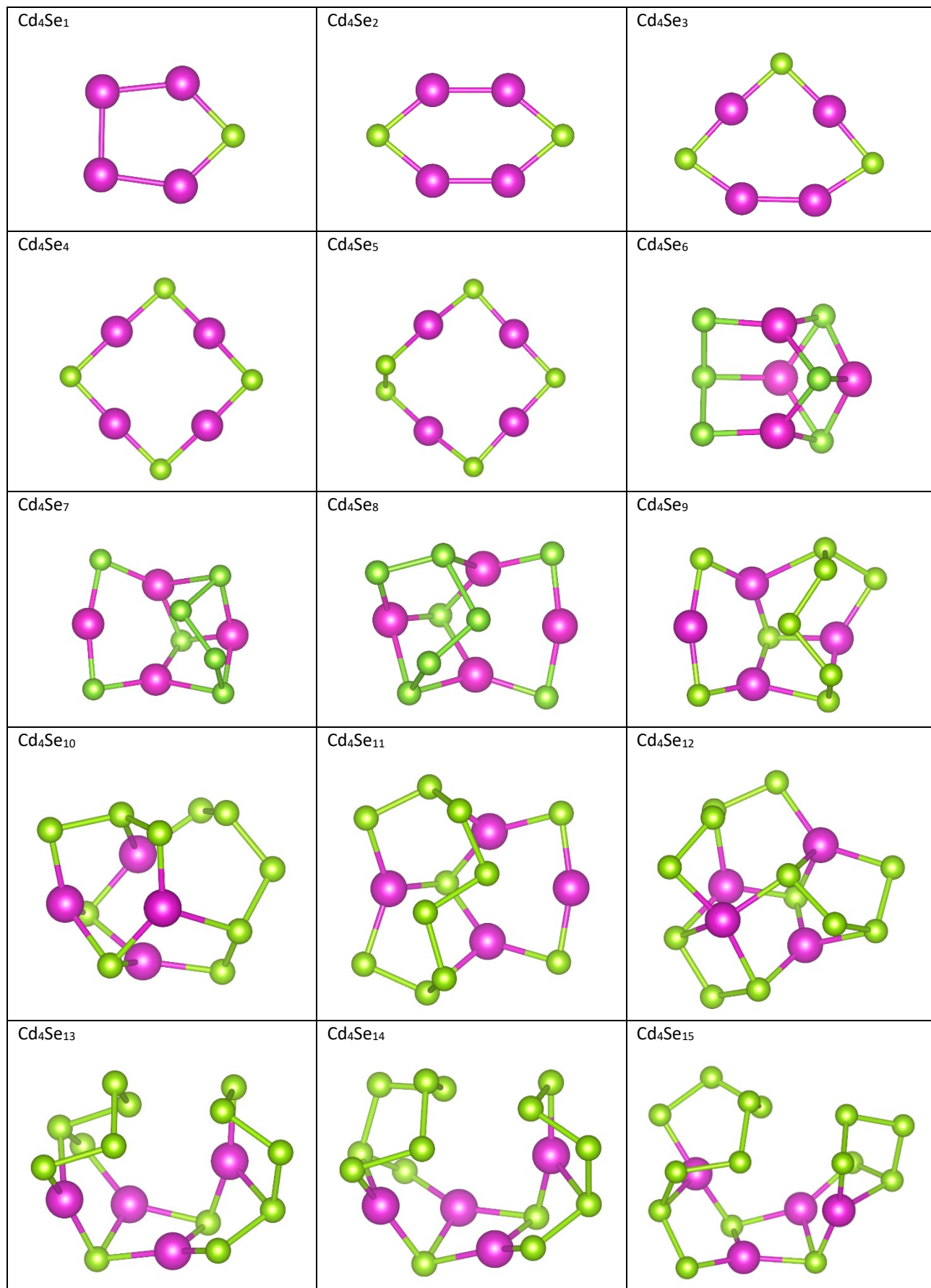[a] correspondence to `v.baturin@skoltech.ru`
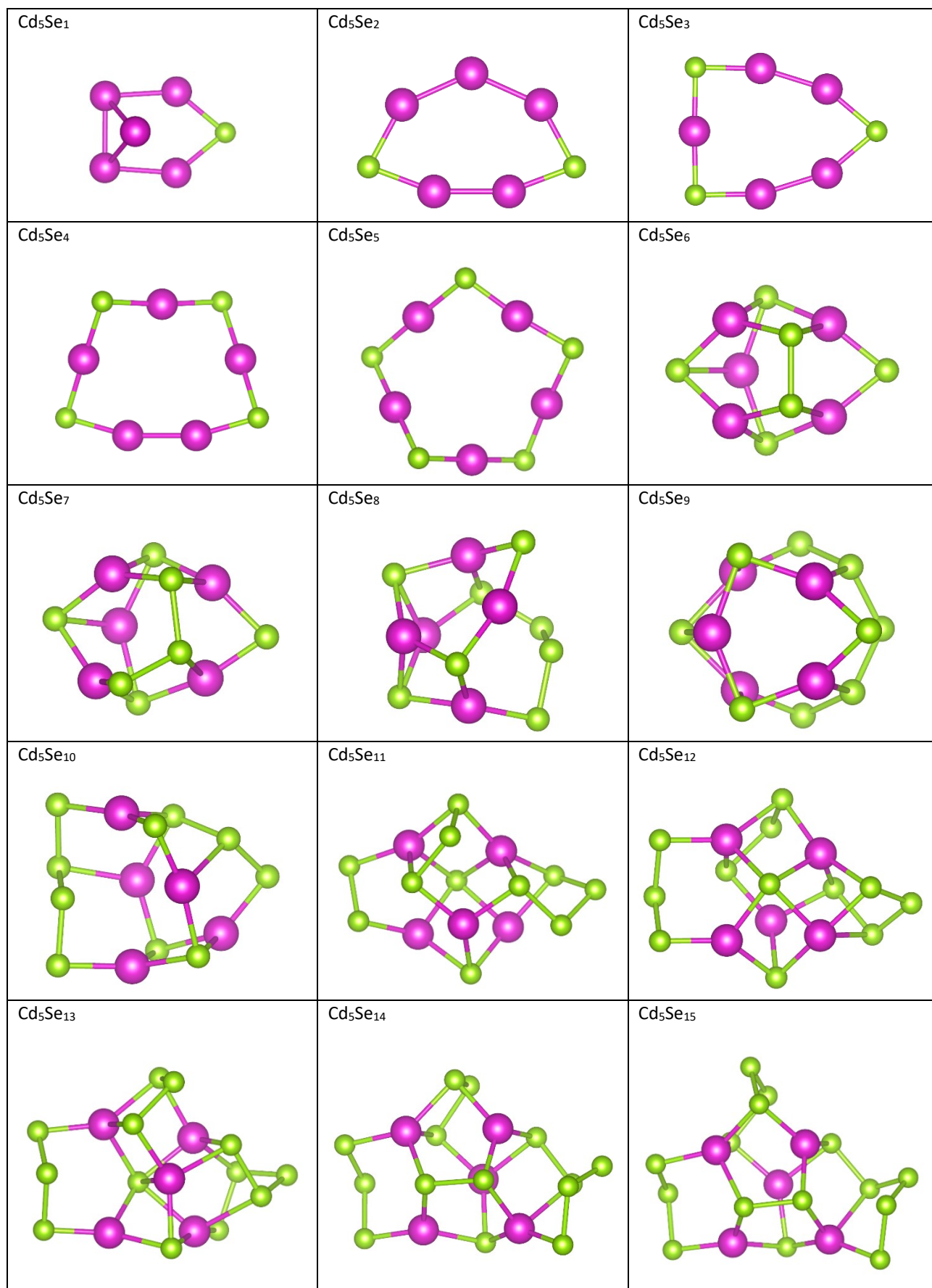
Contents

Table S1 Globally optimized structures of Cd_nSe_m structures ($1 \leq n, m \leq 15$).

Cd_1Se_1	Cd_1Se_2	Cd_1Se_3
Cd_1Se_4	Cd_1Se_5	Cd_1Se_6
Cd_1Se_7	Cd_1Se_8	Cd_1Se_9
Cd_1Se_{10}	Cd_1Se_{11}	Cd_1Se_{12}
Cd_1Se_{13}	Cd_1Se_{14}	Cd_1Se_{15}

Cd$_2$Se$_1$	Cd$_2$Se$_2$	Cd$_2$Se$_3$
Cd$_2$Se$_4$	Cd$_2$Se$_5$	Cd$_2$Se$_6$
Cd$_2$Se$_7$	Cd$_2$Se$_8$	Cd$_2$Se$_9$
Cd$_2$Se$_{10}$	Cd$_2$Se$_{11}$	Cd$_2$Se$_{12}$
Cd$_2$Se$_{13}$	Cd$_2$Se$_{14}$	Cd$_2$Se$_{15}$

Cd$_3$Se$_1$ Cd$_3$Se$_2$ Cd$_3$Se$_3$

Cd$_3$Se$_4$ Cd$_3$Se$_5$ Cd$_3$Se$_6$

Cd$_3$Se$_7$ Cd$_3$Se$_8$ Cd$_3$Se$_9$

Cd$_3$Se$_{10}$ Cd$_3$Se$_{11}$ Cd$_3$Se$_{12}$

Cd$_3$Se$_{13}$ Cd$_3$Se$_{14}$ Cd$_3$Se$_{15}$

Cd_4Se_1	Cd_4Se_2	Cd_4Se_3
Cd_4Se_4	Cd_4Se_5	Cd_4Se_6
Cd_4Se_7	Cd_4Se_8	Cd_4Se_9
Cd_4Se_{10}	Cd_4Se_{11}	Cd_4Se_{12}
Cd_4Se_{13}	Cd_4Se_{14}	Cd_4Se_{15}

Cd_5Se_1	Cd_5Se_2	Cd_5Se_3
Cd_5Se_4	Cd_5Se_5	Cd_5Se_6
Cd_5Se_7	Cd_5Se_8	Cd_5Se_9
Cd_5Se_{10}	Cd_5Se_{11}	Cd_5Se_{12}
Cd_5Se_{13}	Cd_5Se_{14}	Cd_5Se_{15}

Cd_6Se_1

Cd_6Se_2

Cd_6Se_3

Cd_6Se_4

Cd_6Se_5

Cd_6Se_6

Cd_6Se_7

Cd_6Se_8

Cd_6Se_9

Cd_6Se_{10}

Cd_6Se_{11}

Cd_6Se_{12}

Cd_6Se_{13}

Cd_6Se_{14}

Cd_6Se_{15}

Cd$_7$Se$_1$	Cd$_7$Se$_2$	Cd$_7$Se$_3$
Cd$_7$Se$_4$	Cd$_7$Se$_5$	Cd$_7$Se$_6$
Cd$_7$Se$_7$	Cd$_7$Se$_8$	Cd$_7$Se$_9$
Cd$_7$Se$_{10}$	Cd$_7$Se$_{11}$	Cd$_7$Se$_{12}$
Cd$_7$Se$_{13}$	Cd$_7$Se$_{14}$	Cd$_7$Se$_{15}$

Cd$_8$Se$_1$ Cd$_8$Se$_2$ Cd$_8$Se$_3$
Cd$_8$Se$_4$ Cd$_8$Se$_5$ Cd$_8$Se$_6$
Cd$_8$Se$_7$ Cd$_8$Se$_8$ Cd$_8$Se$_9$
Cd$_8$Se$_{10}$ Cd$_8$Se$_{11}$ Cd$_8$Se$_{12}$
Cd$_8$Se$_{13}$ Cd$_8$Se$_{14}$ Cd$_8$Se$_{15}$

Cd$_9$Se$_1$	Cd$_9$Se$_2$	Cd$_9$Se$_3$
Cd$_9$Se$_4$	Cd$_9$Se$_5$	Cd$_9$Se$_6$
Cd$_9$Se$_7$	Cd$_9$Se$_8$	Cd$_9$Se$_9$
Cd$_9$Se$_{10}$	Cd$_9$Se$_{11}$	Cd$_9$Se$_{12}$
Cd$_9$Se$_{13}$	Cd$_9$Se$_{14}$	Cd$_9$Se$_{15}$

$Cd_{10}Se_1$ $Cd_{10}Se_2$ $Cd_{10}Se_3$

$Cd_{10}Se_4$ $Cd_{10}Se_5$ $Cd_{10}Se_6$

$Cd_{10}Se_7$ $Cd_{10}Se_8$ $Cd_{10}Se_9$

$Cd_{10}Se_{10}$ $Cd_{10}Se_{11}$ $Cd_{10}Se_{12}$

$Cd_{10}Se_{13}$ $Cd_{10}Se_{14}$ $Cd_{10}Se_{15}$

Cd₁₁Se₁

Cd₁₁Se₂

Cd₁₁Se₃

Cd₁₁Se₄

Cd₁₁Se₅

Cd₁₁Se₆

Cd₁₁Se₇

Cd₁₁Se₈

Cd₁₁Se₉

Cd₁₁Se₁₀

Cd₁₁Se₁₁

Cd₁₁Se₁₂

Cd₁₁Se₁₃

Cd₁₁Se₁₄

Cd₁₁Se₁₅

Cd$_{12}$Se$_1$	Cd$_{12}$Se$_2$	Cd$_{12}$Se$_3$
Cd$_{12}$Se$_4$	Cd$_{12}$Se$_5$	Cd$_{12}$Se$_6$
Cd$_{12}$Se$_7$	Cd$_{12}$Se$_8$	Cd$_{12}$Se$_9$
Cd$_{12}$Se$_{10}$	Cd$_{12}$Se$_{11}$	Cd$_{12}$Se$_{12}$
Cd$_{12}$Se$_{13}$	Cd$_{12}$Se$_{14}$	Cd$_{12}$Se$_{15}$

$Cd_{13}Se_1$	$Cd_{13}Se_2$	$Cd_{13}Se_3$
$Cd_{13}Se_4$	$Cd_{13}Se_5$	$Cd_{13}Se_6$
$Cd_{13}Se_7$	$Cd_{13}Se_8$	$Cd_{13}Se_9$
$Cd_{13}Se_{10}$	$Cd_{13}Se_{11}$	$Cd_{13}Se_{12}$
$Cd_{13}Se_{13}$	$Cd_{13}Se_{14}$	$Cd_{13}Se_{15}$

Cd$_{14}$Se$_1$	Cd$_{14}$Se$_2$	Cd$_{14}$Se$_3$
Cd$_{14}$Se$_4$	Cd$_{14}$Se$_5$	Cd$_{14}$Se$_6$
Cd$_{14}$Se$_7$	Cd$_{14}$Se$_8$	Cd$_{14}$Se$_9$
Cd$_{14}$Se$_{10}$	Cd$_{14}$Se$_{11}$	Cd$_{14}$Se$_{12}$
Cd$_{14}$Se$_{13}$	Cd$_{14}$Se$_{14}$	Cd$_{14}$Se$_{15}$

$Cd_{15}Se_1$	$Cd_{15}Se_2$	$Cd_{15}Se_3$
$Cd_{15}Se_4$	$Cd_{15}Se_5$	$Cd_{15}Se_6$
$Cd_{15}Se_7$	$Cd_{15}Se_8$	$Cd_{15}Se_9$
$Cd_{15}Se_{10}$	$Cd_{15}Se_{11}$	$Cd_{15}Se_{12}$
$Cd_{15}Se_{13}$	$Cd_{15}Se_{14}$	$Cd_{15}Se_{15}$

Figure S1 Relative stability of Cd$_n$Se$_m$ clusters expressed via lesser of two second-order differences: $E(n, m + 1) + E(n, m - 1) - 2E(n, m)$ and $E(n + 1, m) + E(n - 1, m) - 2E(n, m)$, where $E(n, m)$ is a total energy of Cd$_n$Se$_m$ cluster. As any cluster is globally unstable towards coalescence into the bulk, such a relative stability criteria are used
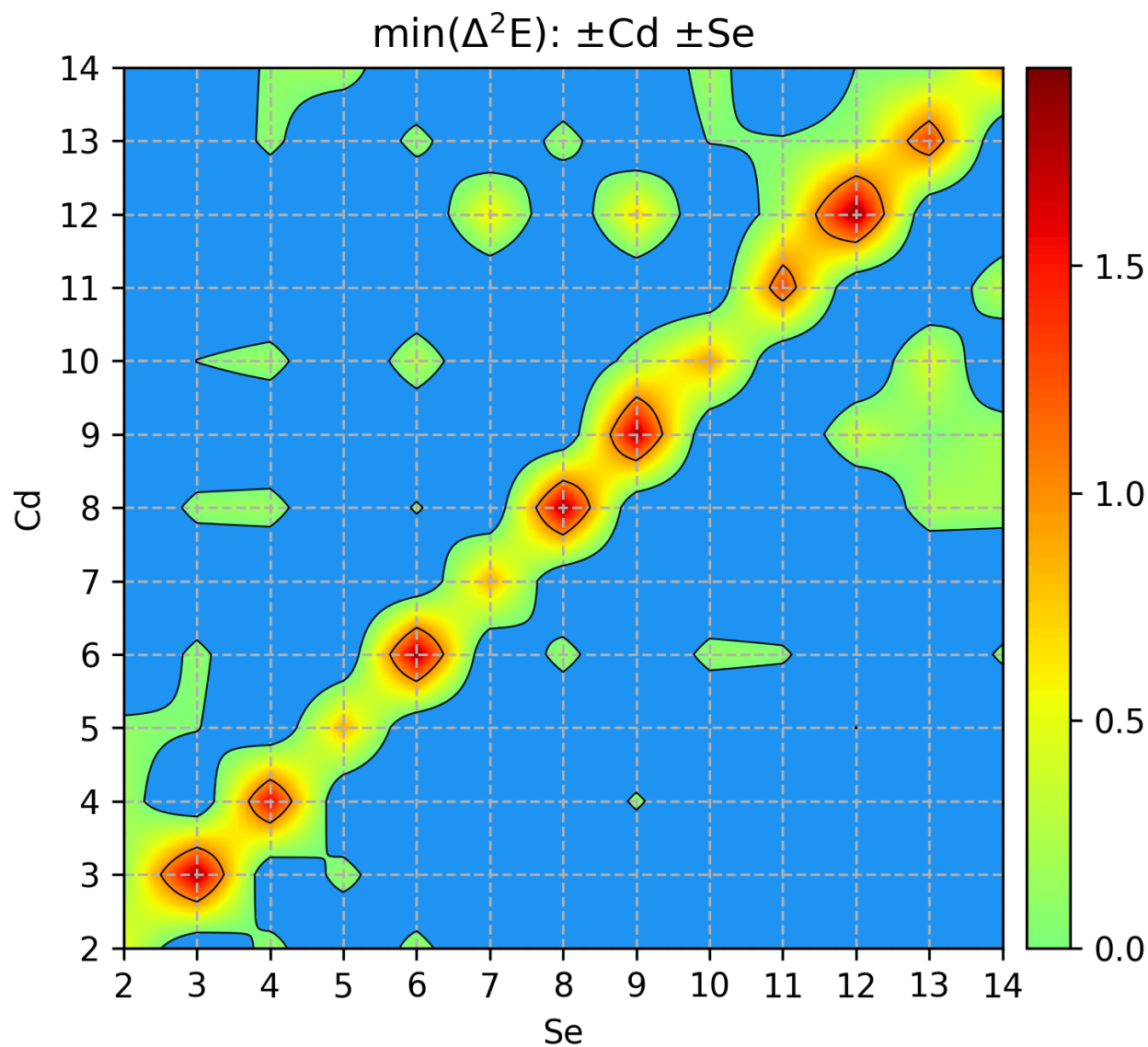
Figure S2 The structure, DOS and IPR = $1/N_{loc}(i)$ of the $Cd_{10}Se_{15}$ (a) and $Cd_{11}Se_{12}$ (b) clusters, corresponding to three stabilization stages
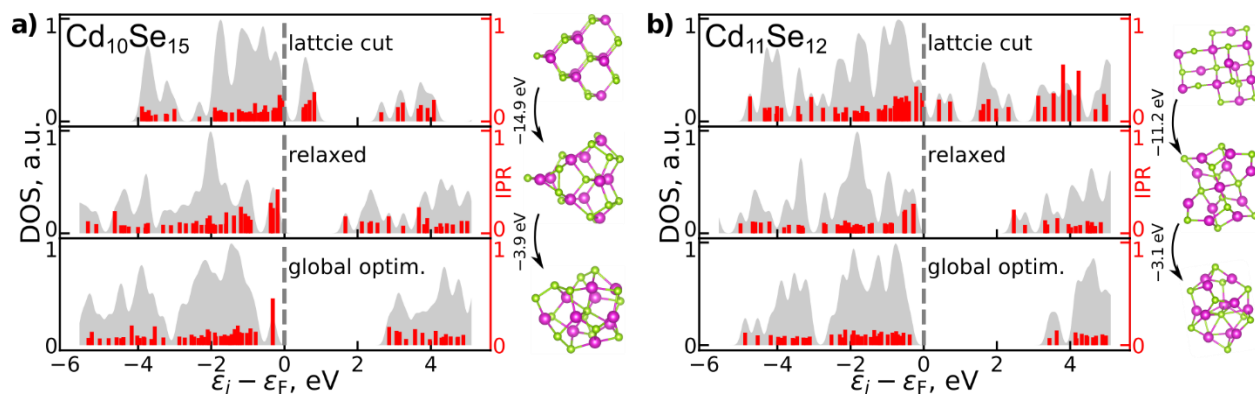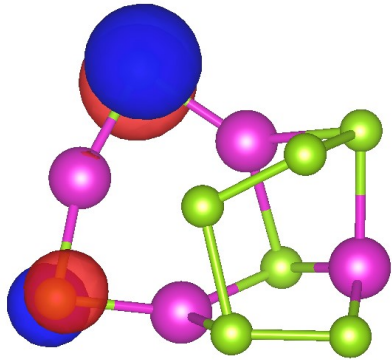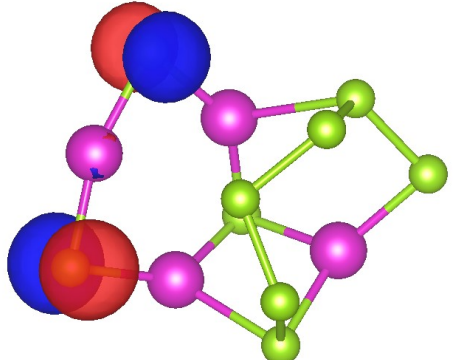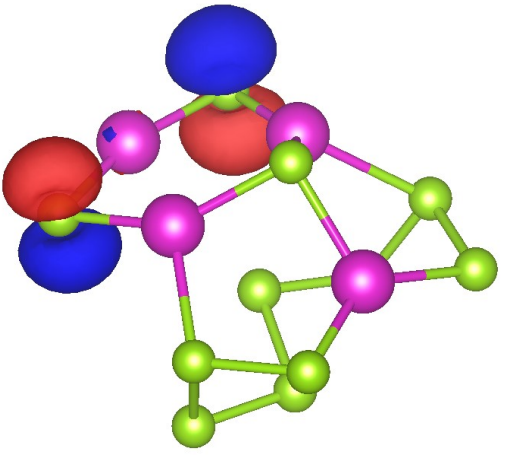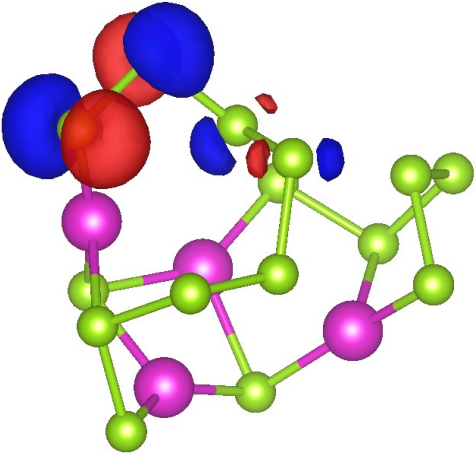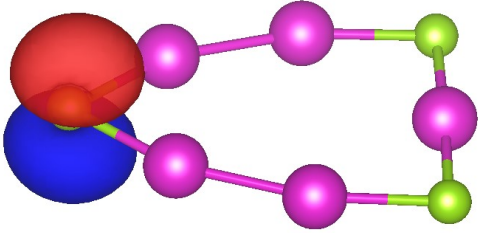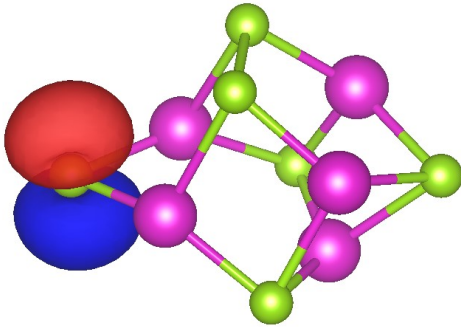
Table S2. Wavefunction, type and localization of strong and medium near-gap traps

Cd$_4$Se$_8$; HOMO; $T^I_a + T^I_a$; N_{loc} = 2.193

Cd$_4$Se$_9$; HOMO; $T^I_a + T^I_a$; N_{loc} = 2.569

Cd$_4$Se$_{11}$; HOMO; $T^I_a + T^I_a$; N_{loc} = 2.754

Cd$_4$Se$_{15}$; HOMO; T^I_c; N_{loc} = 3.360

Cd$_5$Se$_3$; HOMO-1; T^I_a; N_{loc} = 1.388

Cd$_5$Se$_6$; HOMO; T^I_a; N_{loc} = 1.344
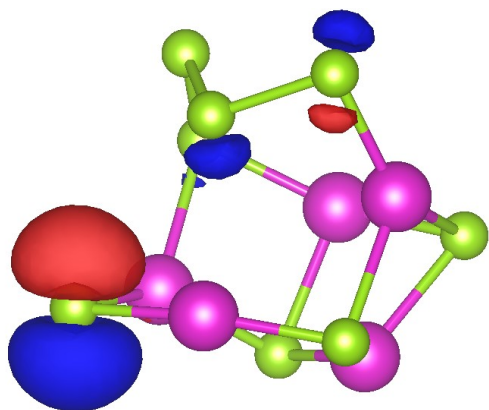
Cd$_5$Se$_8$; HOMO; T^1_a; N_{loc} = 2.220
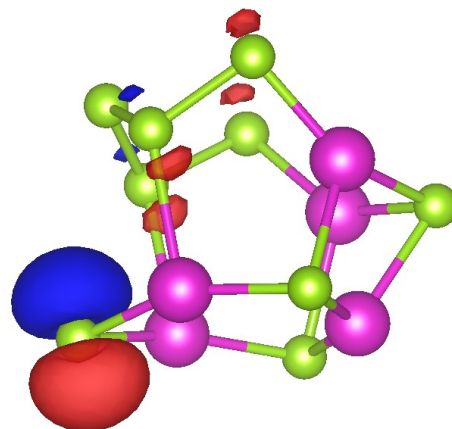
Cd$_5$Se$_9$; HOMO; T^1_a; N_{loc} = 2.644
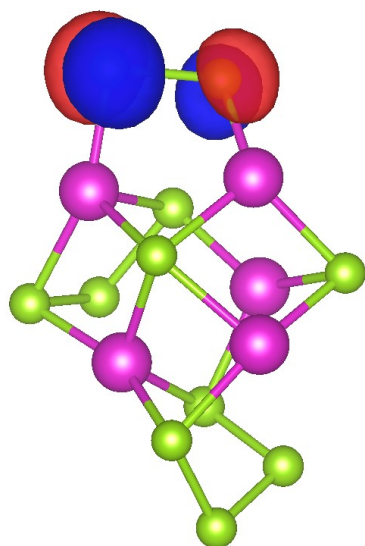
Cd$_5$Se$_{11}$; HOMO; T^1_c; N_{loc} = 2.394
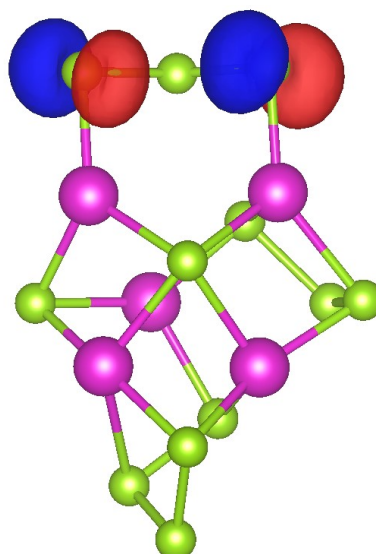
Cd$_5$Se$_{12}$; HOMO; $T^1_a + T^1_a$; N_{loc} = 2.796
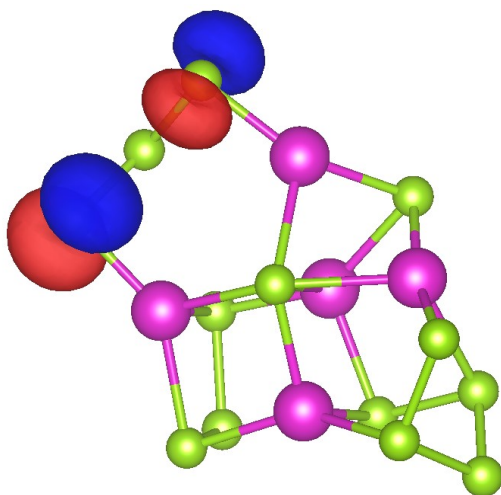
Cd$_5$Se$_{13}$; HOMO - 1 ; $T^1_a + T^1_a$; N_{loc} = 3.514
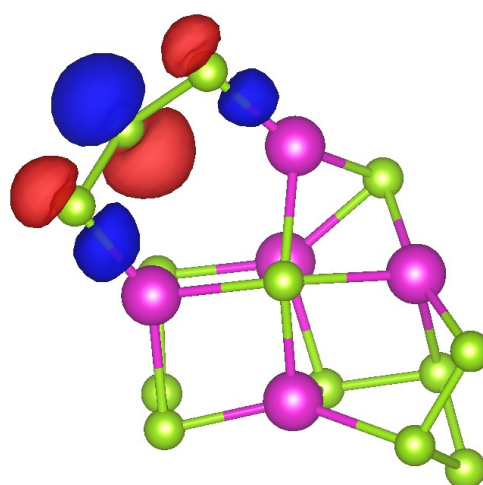
Cd$_5$Se$_{13}$; HOMO; T^1_d; N_{loc} = 2.519
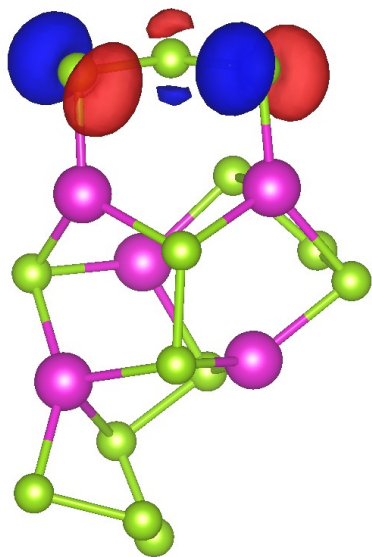
Cd$_5$Se$_{14}$; HOMO - 1; $T^1_a + T^1_a$; N_{loc} = 3.698
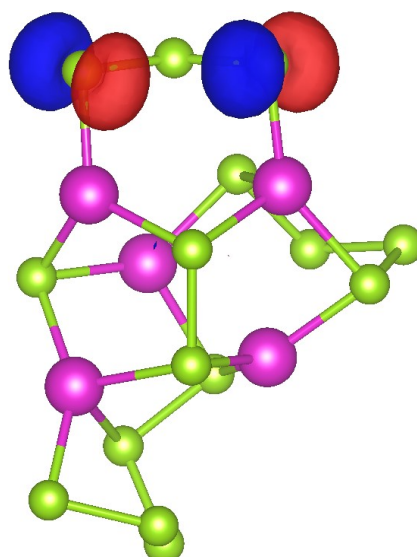
Cd$_5$Se$_{15}$; HOMO - 1; $T^1_a + T^1_a$; N_{loc} = 3.098
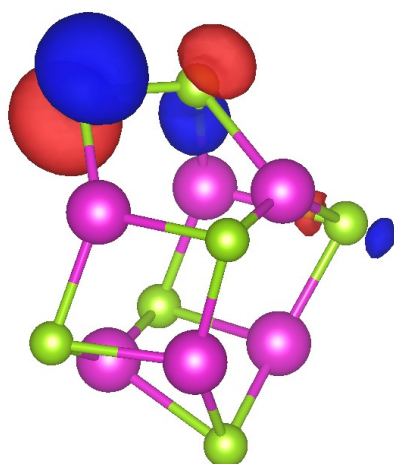
Cd$_6$Se$_7$; HOMO; T^1_b; N_{loc} = 2.374
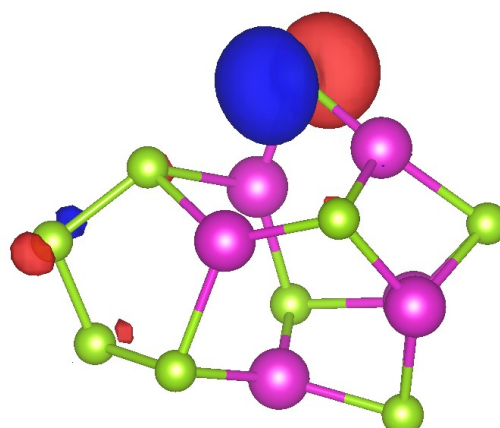
Cd$_6$Se$_9$; HOMO; T^1_a; N_{loc} = 2.085
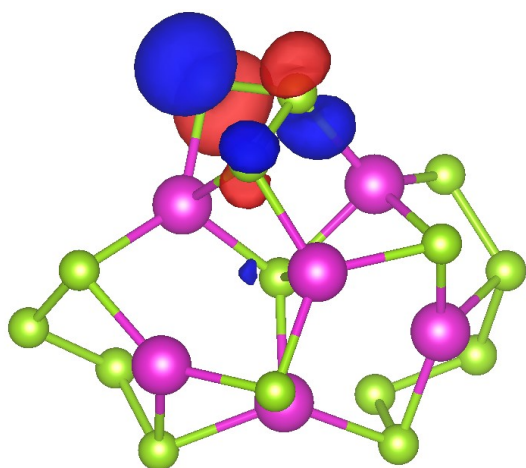
Cd$_6$Se$_{15}$; HOMO; T^1_b; N_{loc} = 2.719
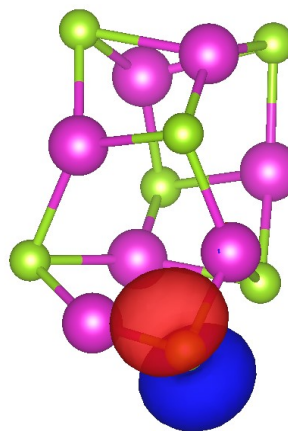
Cd$_7$Se$_7$; HOMO; T^1_a; N_{loc} = 1.584
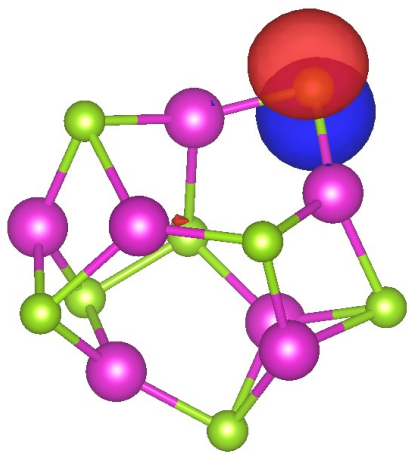
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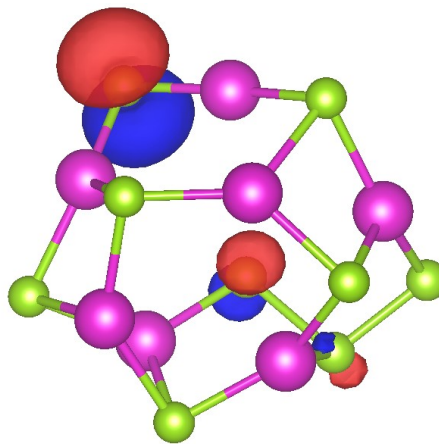
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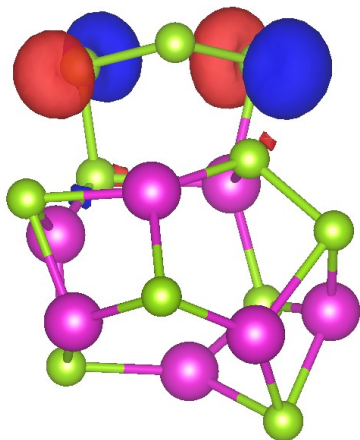
Cd$_7$Se$_{11}$; HOMO - 1; $T^1_a + T^1_a$; N_{loc} = 3.339
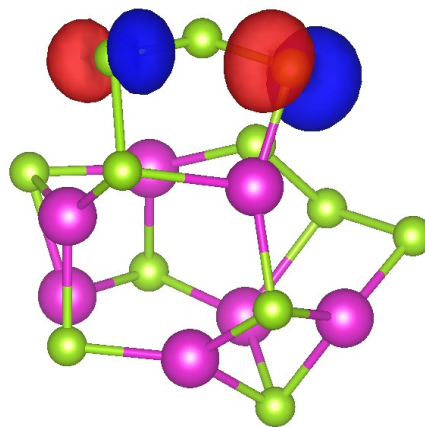
Cd$_7$Se$_{12}$; HOMO - 1; $T^1_a + T^1_a$; N_{loc} = 3.059
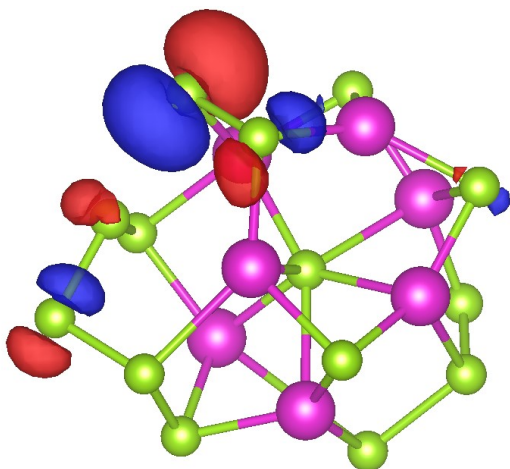
Cd$_7$Se$_{15}$; HOMO; T^1_b; N_{loc} = 2.728
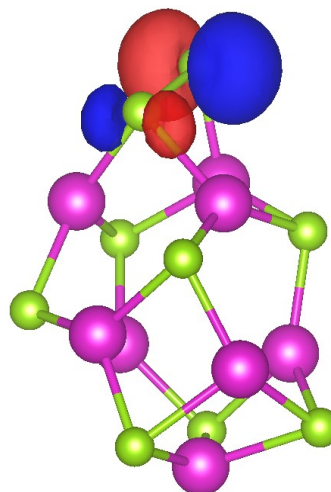
Cd$_8$Se$_9$; HOMO; T^1_b; N_{loc} = 1.747
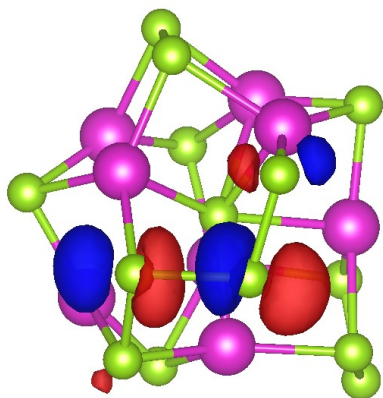
Cd$_8$Se$_{14}$; LUMO; T^{II}_b; $N_{loc} = 3.942$
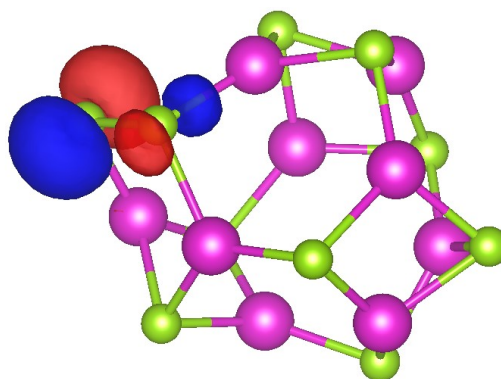
Cd$_9$Se$_{10}$; HOMO; T^{I}_b; $N_{loc} = 2.053$
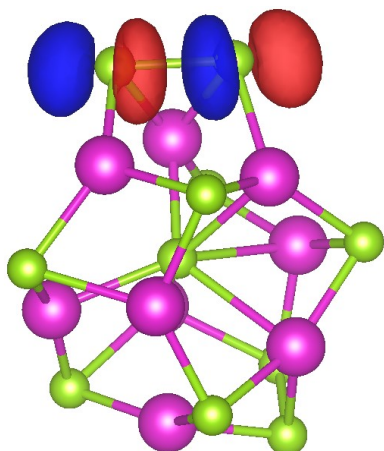
Cd$_9$Se$_{11}$; LUMO + 1; T^{II}_a; $N_{loc} = 3.906$
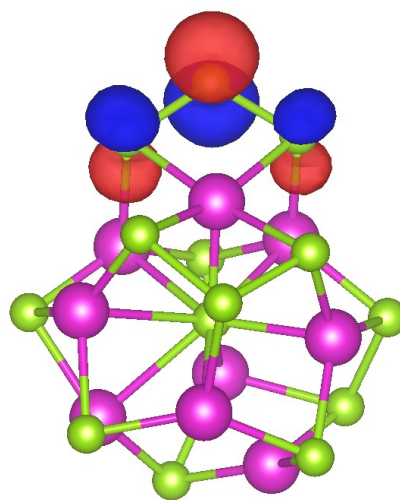
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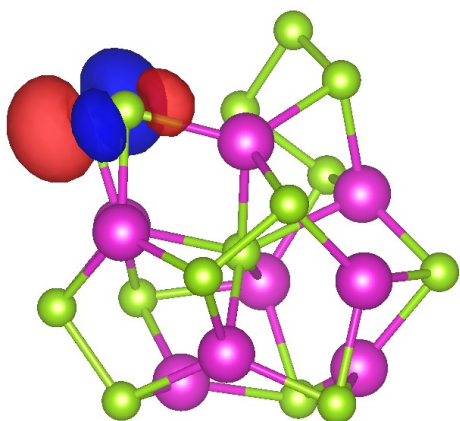
Cd$_9$Se$_{15}$; HOMO; T^{I}_b; $N_{loc} = 2.140$
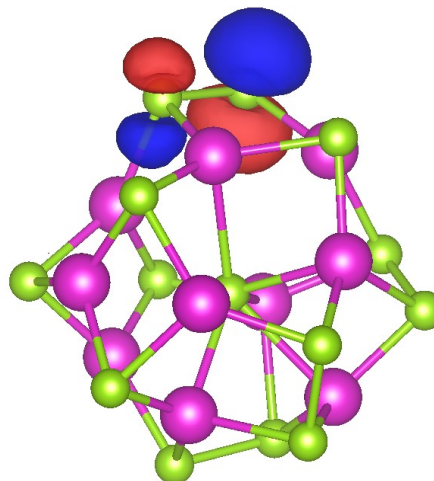
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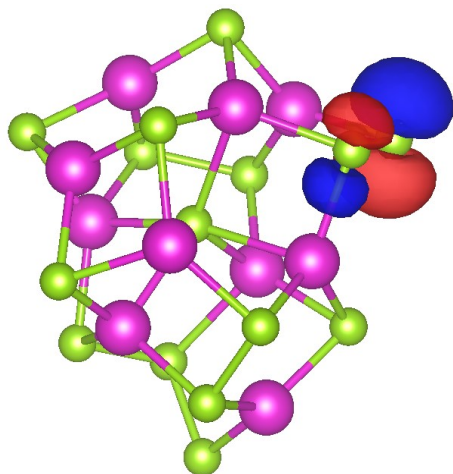
Cd$_{10}$Se$_{15}$; HOMO; T^{I}_b; N_{loc} = 2.177
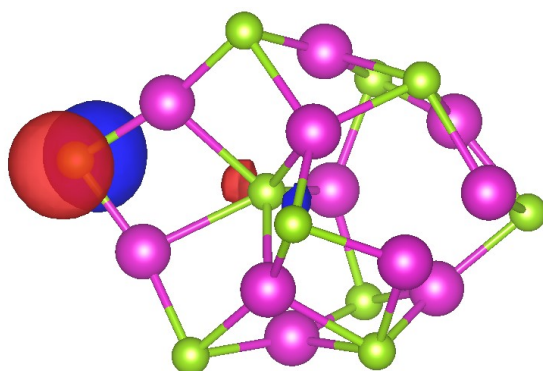
Cd$_{11}$Se$_{10}$; HOMO - 1; T^{I}_a; N_{loc} = 1.728
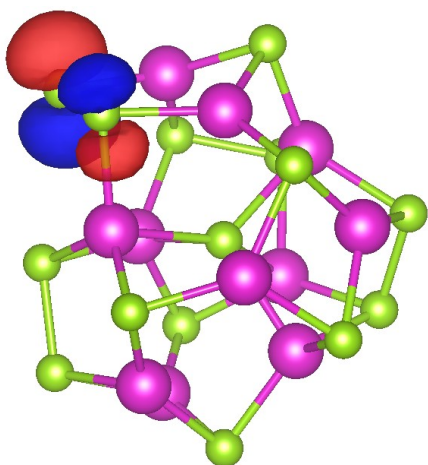
Cd$_{11}$Se$_{15}$; HOMO; T^{I}_b; N_{loc} = 2.664
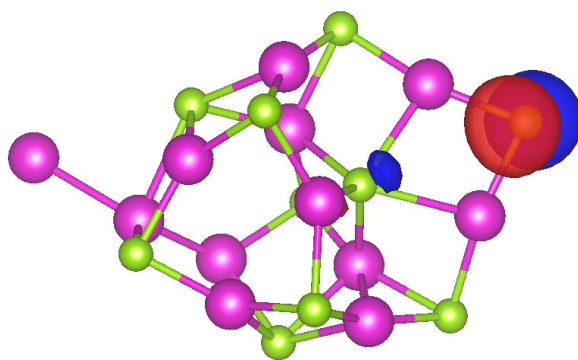
Cd$_{12}$Se$_{10}$; HOMO - 1; T^{I}_a; N_{loc} = 1.781
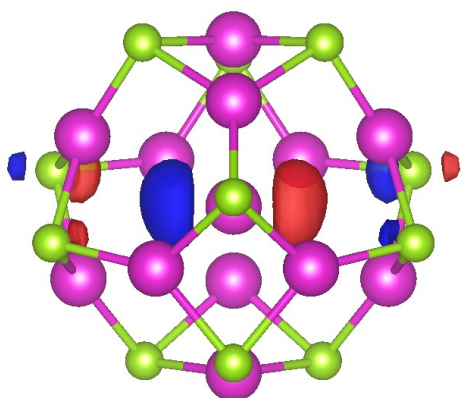
Cd$_{13}$Se$_{11}$; LUMO + 1; T^{III}; N_{loc} = 2.959
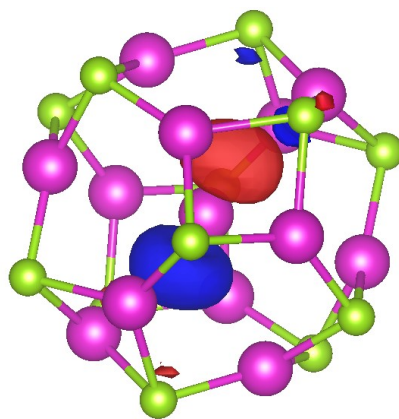
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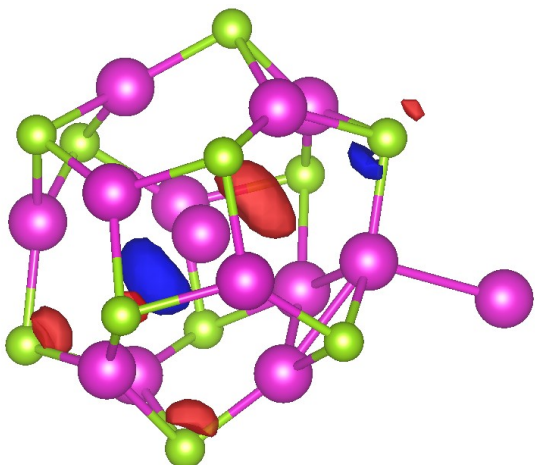
Cd$_{14}$Se$_{11}$; LUMO + 1; T^{III}; N_{loc} = 3.744
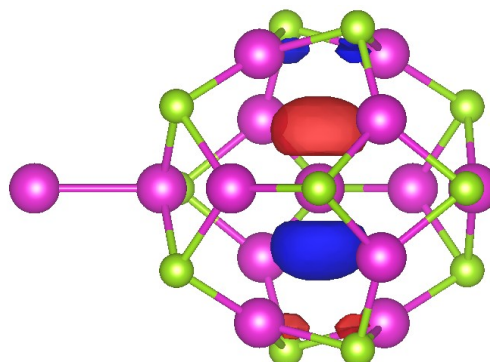
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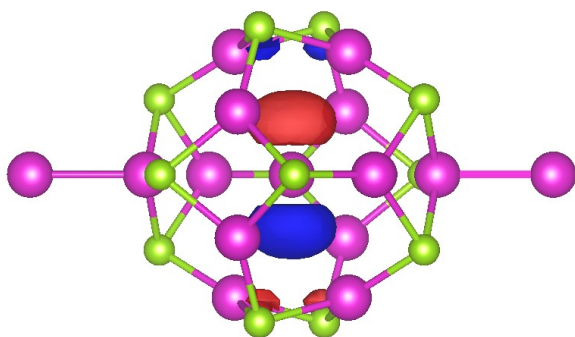
Cd$_{15}$Se$_{12}$; LUMO + 1; T^{III}; N_{loc} = 2.195