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Structures and stability of small bimetallic In–Pd and Ag–Pd clusters: a DFT investigation

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S1. Absolute energies and Cartesian coordinates for investigated clusters

Geometry optimizations and vibrational frequency analysis were performed using PBE and Λ_2 basis set.

Pd_4
E = -20185.492638412 a.u.

46	-1.336079780	-0.843000210	0.076703990
46	1.244500690	-0.934249500	-0.282852190
46	0.146843500	0.733735940	1.393459350
46	-0.055264400	1.043513780	-1.187000000

$InPd_3$
E = -21021.468190907 a.u.

46	-1.160929710	0.918505000	-0.534758990
46	-0.602419270	-0.843183220	1.184681060
46	0.335505600	-1.018302800	-1.152331960
49	1.427843390	0.942981010	0.502409890

In_2Pd_2
E = -21857.442220220 a.u.

46	1.785914350	-0.056669300	-1.077851850
49	0.750441380	-0.406280370	1.264781790
49	-0.750441230	0.406280320	-1.264781820
46	-1.785914500	0.056669350	1.077851880

In_3Pd
E = -22693.358176061 a.u.

46	-0.640960760	0.668218390	-1.081637330
49	-0.752894280	0.804872540	1.568093390
49	-0.469903280	-1.843391360	-0.235770530
49	1.863758320	0.370300430	-0.250685530

In_4

E = -23529.227219678 a.u.

49	-0.982902960	2.447692980	-0.448279010
49	0.498250980	-0.077885410	-1.517788970
49	-0.498259640	0.077885960	1.517816610
49	0.982911620	-2.447693530	0.448251370

$AgPd_3$

E = -20455.695844024 a.u.

46	-1.282474160	0.922035150	0.143112890
46	0.656806870	0.280794830	-1.415966510
46	1.040143880	0.420237810	1.121056580
47	-0.414476580	-1.623067790	0.151797040

Ag_2Pd_2

E = -20725.890328812 a.u.

47	-0.904945680	1.137822260	-0.822043030
46	0.904748110	-0.782387230	-1.083004500
46	0.904881420	0.782471700	1.082833230
47	-0.904683850	-1.137906730	0.822214310

Ag_3Pd

E = -20996.072557629 a.u.

47	-0.590650230	1.206392150	0.034318440
47	-0.283437650	-0.096376960	-2.308472320
47	0.442403150	0.128416040	2.281766370
46	0.431684730	-1.238431230	-0.007612500

Ag_4

E = -21266.271122449 a.u.

47	-1.801251480	-1.316157650	-0.903731240
47	-0.284917550	0.961310900	-0.832138410
47	1.801259500	1.316152230	0.903723160
47	0.284909540	-0.961305470	0.832146480

S2. Hirshfeld charges

Hirsfeld charges calculations were performed using PBE and Λ_2 basis set.

Table S1 Calculated Hirshfeld charges of Pd and In in In_nPd_{4-n} clusters (n = 0-4).

Cluster	Atom type and Hirshfeld charge			
Pd_4	-0.01 (Pd_1)	-0.01 (Pd_2)	-0.01 (Pd_3)	-0.01 (Pd_4)
$InPd_3$	-0.07 (Pd_1)	-0.07 (Pd_2)	-0.07 (Pd_3)	0.19 (In_4)
In_2Pd_2	-0.26 (Pd_1)	0.26 (In_2)	0.26 (In_3)	-0.26 (Pd_4)
In_3Pd	-0.34 (Pd_1)	0.11 (In_2)	0.11 (In_3)	0.11 (In_4)
In_4	0.05 (In_1)	-0.05 (In_2)	-0.05 (In_3)	0.05 (In_4)

Table S2 Calculated Hirshfeld charges of Pd and Ag in Ag_nPd_{4-n} clusters (n = 0-4).

Cluster	Atom type and Hirshfeld charge			
Pd_4	-0.01 (Pd_1)	-0.01 (Pd_2)	-0.01 (Pd_3)	-0.01 (Pd_4)
$AgPd_3$	-0.04 (Pd_1)	-0.04 (Pd_2)	-0.04 (Pd_3)	0.11 (Ag_4)
Ag_2Pd_2	0.09 (Ag_1)	-0.10 (Pd_2)	-0.10 (Pd_3)	0.09 (Ag_4)
Ag_3Pd	0.07 (Ag_1)	0.01 (Ag_2)	0.01 (Ag_3)	-0.09 (Pd_4)
Ag_4	-0.10 (Ag_1)	0.10 (Ag_2)	-0.10 (Ag_3)	0.10 (Ag_4)