

## Supporting Information: ‘Structural and electronic properties for Be-doped Pt<sub>n</sub> (n = 1 – 12) clusters obtained by DFT calculations’

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# 1 Formulas and Definitions for the Energetic Parameters

## 1.1 Binding energy and fragmentation energy

The stability of  $Pt_nBe$  clusters (with  $n = 1 - 12$ ) is investigated by calculating the binding energy per atom ( $E_B$ ), and fragmentation energy ( $E_f$ ), defined as

$$E_B[Pt_nBe] = \{E[Be] + nE[Pt] - E[Pt_nBe]\}/n, \quad (1)$$

$$E_f[Pt_nBe] = E[Pt_{n-1}Be] + \{E[Pt] + E[Be]\} - E[Pt_nBe], \quad (2)$$

where  $E[Be]$ ,  $E[Pt]$ , and  $E[Pt_nBe]$  are the total energies of the bare Be atom, the Pt atom, and the  $Pt_nBe$  doped cluster.

## 1.2 Ionization potential and electron affinity

The vertical ionization potential (vIP) and vertical electron affinity (vEA) are calculated as follows:

$$vIP = E[Pt_nBe^+] - E[Pt_nBe], \quad (3)$$

$$vEA = E[Pt_nBe] - E[Pt_nBe^-]. \quad (4)$$

## 1.3 Chemical Hardness

The chemical hardness is approximated as

$$\eta \approx \frac{1}{2}(vIP - vEA). \quad (5)$$

## 1.4 The d-band center

The position of the d-band center  $\epsilon_d$  is calculated by the following expression:

$$\epsilon_d = \frac{\sum_i \epsilon_i * d(\epsilon_i)}{\sum_i d(\epsilon_i)}, \quad (6)$$

since the clusters studied in this work have a magnetic character, we have included the d-band center ( $\epsilon_d$ ) of the clusters for the majority ( $\epsilon_d \uparrow$ ) and minority spin states ( $\epsilon_d \downarrow$ ), respectively.

# 2 Cartesian coordinates

## 2.1 The lowest energy structures of $Pt_nBe$ ( $n = 3 - 12$ ) clusters calculated using the G09 program and the PW91/cc-pVDZ-PP approach.

### Pt<sub>3</sub>Be geometry:

Be	-0.000001000	-1.234163000	0.000258000
Pt	1.925534000	-0.517061000	-0.000010000
Pt	-1.925534000	-0.517061000	-0.000010000
Pt	0.000000000	1.097412000	0.000006000

### Pt<sub>4</sub>Be geometry:

Be	-0.001054000	1.241594000	0.000000000
Pt	1.306255000	-0.553340000	0.000000000
Pt	-0.001054000	0.523493000	2.031748000
Pt	-0.001054000	0.523493000	-2.031748000
Pt	-1.304092000	-0.557317000	0.000000000

### Pt<sub>5</sub>Be geometry:

Be	0.084593000	-0.000123000	-1.032906000
Pt	-0.637818000	-1.330849000	0.747918000

Pt	-0.638505000	1.330982000	0.747660000
Pt	1.692327000	-1.300584000	-0.274389000
Pt	-2.112049000	-0.000531000	-0.893733000
Pt	1.691708000	1.300988000	-0.274486000

**Pt<sub>6</sub>Be geometry:**

Be	-0.505396000	0.000092000	-1.157669000
Pt	0.694622000	-1.710450000	-0.619674000
Pt	-1.963340000	1.305026000	-0.065373000
Pt	-1.963404000	-1.304930000	-0.065301000
Pt	0.071963000	0.000000000	1.234397000
Pt	0.694851000	1.710469000	-0.619593000
Pt	2.491226000	-0.000119000	0.194911000

**Pt<sub>7</sub>Be geometry:**

Be	-0.952840000	0.000038000	-1.114097000
Pt	0.719743000	0.000086000	1.510027000
Pt	0.815761000	-1.354149000	-0.688753000
Pt	2.909226000	-0.000193000	0.007710000
Pt	-1.678156000	2.013525000	-0.546757000
Pt	0.816011000	1.354048000	-0.688930000
Pt	-1.678459000	-2.013391000	-0.546778000
Pt	-1.855263000	0.000074000	1.010615000

**Pt<sub>8</sub>Be geometry:**

Be	0.915059000	0.884257000	0.874227000
Pt	-0.543521000	-0.902424000	1.406716000
Pt	-2.765039000	-0.853898000	-0.027539000
Pt	0.591785000	2.964225000	0.207579000
Pt	0.519750000	0.896374000	-1.350984000
Pt	-1.407011000	1.309265000	0.284770000
Pt	2.046026000	-1.117981000	-1.015892000
Pt	-0.513243000	-1.479847000	-1.101039000
Pt	2.024326000	-0.861061000	1.551557000

**Pt<sub>9</sub>Be geometry:**

Be	0.761679000	1.179710000	0.000000000
Pt	2.072611000	-0.475831000	0.000000000
Pt	-0.283427000	-1.156861000	1.360371000
Pt	-0.283427000	-1.156861000	-1.360371000
Pt	-2.416626000	-1.063145000	0.000000000
Pt	1.769589000	-0.198389000	-2.541636000
Pt	1.769589000	-0.198389000	2.541636000
Pt	-0.283427000	1.332218000	-1.827853000
Pt	-0.283427000	1.332218000	1.827853000
Pt	-2.100518000	1.524540000	0.000000000

**Pt<sub>10</sub>Be geometry:**

Be	-0.353038000	0.754351000	1.396679000
Pt	2.429198000	0.049364000	-0.149070000
Pt	1.390201000	-0.907221000	-2.308712000

Pt	-0.354155000	-2.168297000	-0.839838000
Pt	0.667371000	-1.151599000	1.225088000
Pt	1.789803000	0.999174000	2.259803000
Pt	0.697407000	1.908605000	-0.088590000
Pt	-1.795964000	-2.022125000	1.319067000
Pt	-0.757287000	0.261932000	-1.377666000
Pt	-2.326580000	0.406997000	0.607749000
Pt	-1.721891000	2.584484000	-0.719456000

**Pt<sub>11</sub>Be geometry:**

Be	0.036771000	0.144637000	0.000000000
Pt	-2.358484000	-1.951366000	0.000000000
Pt	0.066503000	-1.710036000	1.295600000
Pt	1.695516000	0.314410000	1.464270000
Pt	-1.722643000	0.206236000	1.389666000
Pt	2.500097000	-1.724504000	0.000000000
Pt	-0.106430000	1.867858000	2.518570000
Pt	0.066503000	-1.710036000	-1.295600000
Pt	-1.722643000	0.206236000	-1.389666000
Pt	-0.009391000	2.311515000	0.000000000
Pt	1.695516000	0.314410000	-1.464270000
Pt	-0.106430000	1.867858000	-2.518570000

**Pt<sub>12</sub>Be geometry:**

Be	0.143971000	-1.187226000	0.874013000
Pt	-3.076122000	-0.565066000	-0.894169000
Pt	-1.566148000	-2.573849000	0.073415000
Pt	-1.743486000	1.642901000	-0.866473000
Pt	0.203903000	1.834507000	1.113399000
Pt	-1.744135000	-0.156883000	1.324798000
Pt	0.148530000	0.203263000	3.052934000
Pt	-0.399216000	-0.442768000	-1.320559000
Pt	0.355242000	3.076333000	-1.093398000
Pt	1.718380000	0.918858000	-1.165294000
Pt	0.934885000	-2.502171000	-0.738239000
Pt	2.025992000	-0.202626000	1.297113000
Pt	3.134791000	-1.171616000	-0.828349000