



## Supporting Information

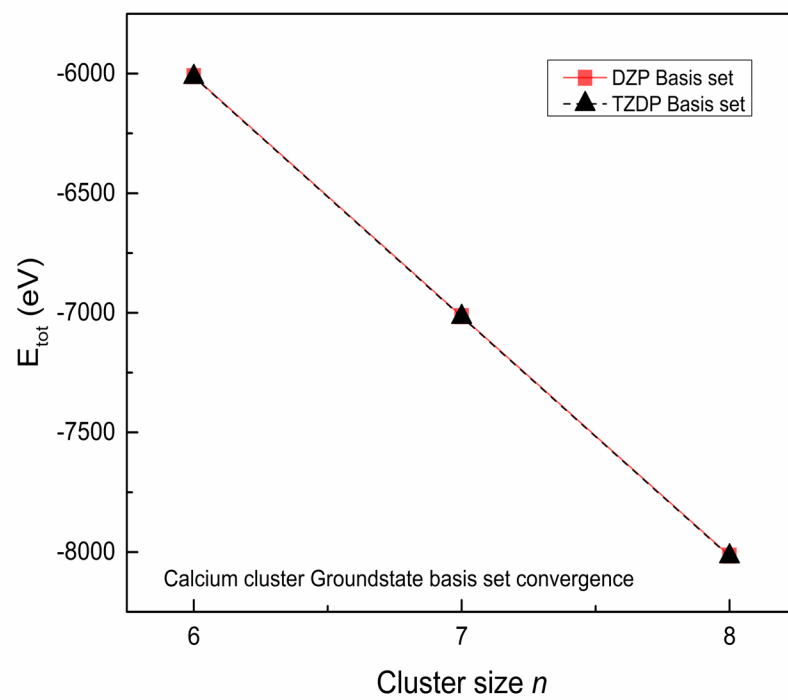
for

### **Ca<sub>n</sub> neutral clusters: a two-step G<sub>0</sub>W<sub>0</sub> and DFT benchmark**

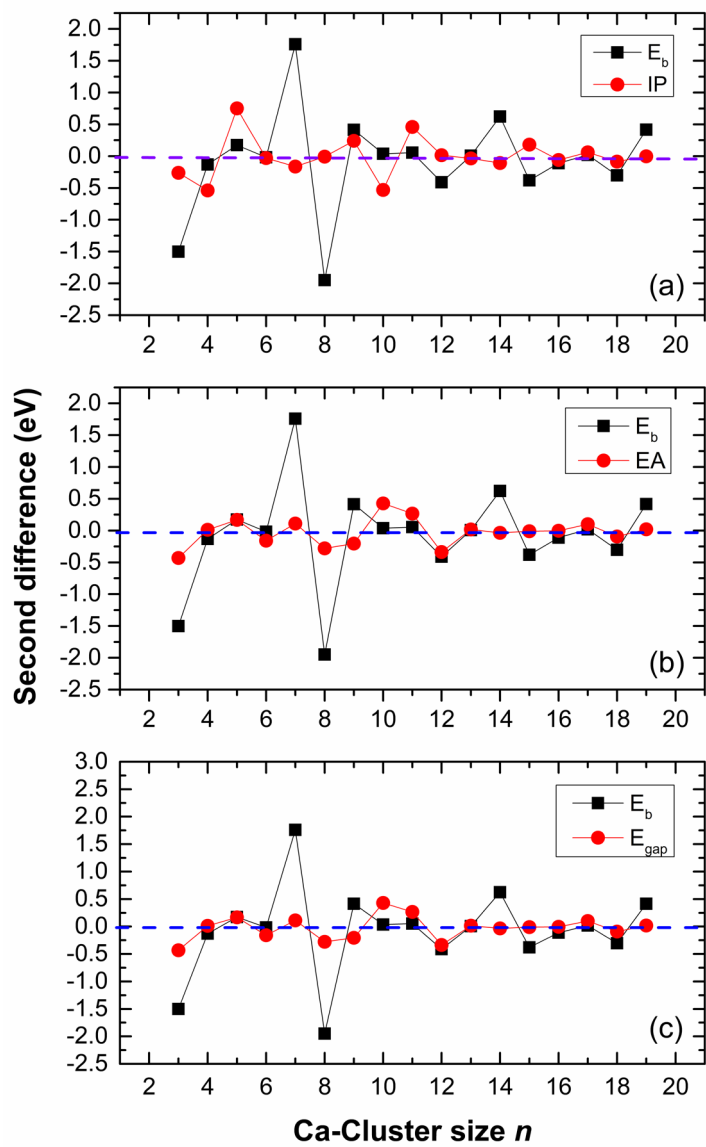
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## Additional experimental data



**Figure S1:** The DZP and TZDP basis set convergence results of the total energy of ground state calcium clusters for size  $n = 6-8$ .



**Figure S2:** The second difference of energy for  $E_b$  versus a) IP, b) EA and, c)  $E_{gap}$ .

**The ground state geometry files are provided in XYZ format below:**

3:

```
atom 10.833176065055  10.317750000000  12.144787498620 Ca
atom 9.664883925490  12.180606632466  9.137200534686 Ca
atom 9.664883925490  8.454893367535  9.137200534685 Ca
```

4:

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atom 8.960168136790  11.532807783015  8.960106654168 Ca
atom 11.532744417006  8.960241207357  8.960241206972 Ca
atom 11.532724238207  11.532444355830  11.532444355416 Ca
atom 8.960168135992  8.960106653797  11.532807783443 Ca
```

5:

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atom 5.580859737505  5.504299999975  8.499691822744 Ca
atom 5.580859281894  5.504299999972  1.999348074752 Ca
atom 3.532854309305  5.504300000007  5.249521551292 Ca
atom 6.608578748135  3.720961914433  5.249521770605 Ca
atom 6.608578748145  7.287638085539  5.249521770604 Ca
```

6:

```
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atom 5.028515091569  5.066023558045  7.266071046153 Ca
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atom 5.518779752617  8.312453441437  5.509800508595 Ca
atom 8.290376714087  5.388440321591  5.506494041479 Ca
atom 1.863344384364  6.344698220586  5.514633393965 Ca
```

7:

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atom 8.651208030106  4.443866790440  5.463617771039 Ca
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atom 3.571795414352 8.064615271018 5.461401060691 Ca

8:

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atom 12.810226348983 12.856075908408 15.421607725608 Ca  
atom 10.693425097439 9.897324924124 16.175893584205 Ca  
atom 16.094001522032 11.957250827966 13.712052307584 Ca  
atom 10.003112123166 11.867326085884 13.102865102252 Ca

9:

atom 10.385602086230 9.961683368563 11.783025201576 Ca  
atom 7.257640539800 11.782479099888 12.228007507681 Ca  
atom 7.261688881845 8.224259301521 11.057752872286 Ca  
atom 13.511478371425 8.226374931814 11.062706934255 Ca  
atom 13.511566143155 11.784928622459 12.232393846185 Ca  
atom 10.385032705395 13.464983898157 10.865410510420 Ca  
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atom 12.249271095435 10.930455582960 8.839795590249 Ca

10:

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atom 8.353944660128 12.630375835397 9.404772051386 Ca  
atom 10.492632112017 10.492757247144 7.158166156144 Ca

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11:

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13:

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14:

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19:

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