A comparative study on the interaction of platinum with group 4A (germanium, tin and lead) porphyrins*

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Calculations:
- Targets: SnPor-Pt, GePor-Pt, PbPor-Pt
- Density functional theory, Gaussian03.
- LANL2DZ basis set and B3LYP exchange-correlation functionals.
- Confirmed ground states
- Full geometry relaxation.

Results:

<table>
<thead>
<tr>
<th>M-Pt (Å)</th>
<th>GePor-Pt</th>
<th>SnPor-Pt</th>
<th>PbPor-Pt</th>
</tr>
</thead>
<tbody>
<tr>
<td>M-Pt (Å)</td>
<td>2.283</td>
<td>2.418</td>
<td>2.472</td>
</tr>
<tr>
<td>Binding E (eV)</td>
<td>3.13!</td>
<td>3.13!</td>
<td>1.99</td>
</tr>
</tbody>
</table>

Conclusion:
- Pt deposits very stably on SnPor and GePor.
- The localization of HOMO/near HOMO electrons on Pt (to be shown in detail during session)
- Dispersing Pt on SnPor and GePor may be a good way to reduce platinum load in catalysts.