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

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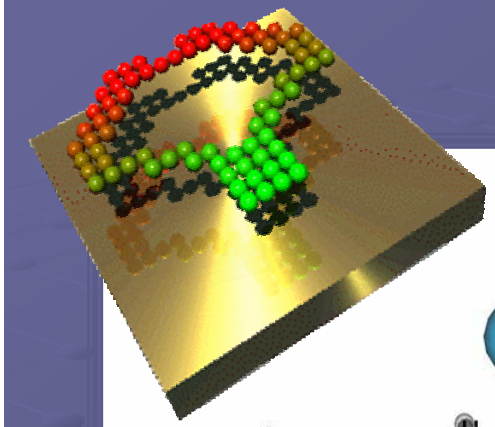
EBEN S. DY and HIDEAKI KASAI

Kasai Laboratory, Department of Applied Physics, Osaka University



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:	GePor-Pt	SnPor-Pt	PbPor-Pt
M-Pt (Å)	2.283	2.418	2.472
Binding E (eV)	3.13!	3.13!	1.99

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.