Objective: develop a systematic *ab initio* modeling strategy to understand structure-property relationships in *amorphous* catalysts and supports

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principles for modeling amorphous supports with cluster models

(1) support is a solid so peripheral atoms should be immobile.
(2) peripheral atom positions (x_p) influence chemical properties of the site.
(3) peripheral atoms arranged in continuous distribution of positions.
(4) low energy sites are more prevalent than high energy sites.

(1-4) define the most prevalent model sites for each value of each property. Find them with sequential quadratic programming.

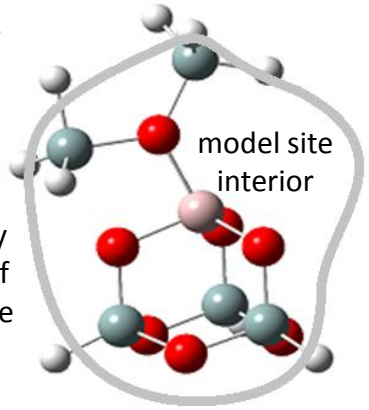
$$g^A_{p,eff} = g^A_p - H_{pa} H^{-1}_{aa} g^A_a$$

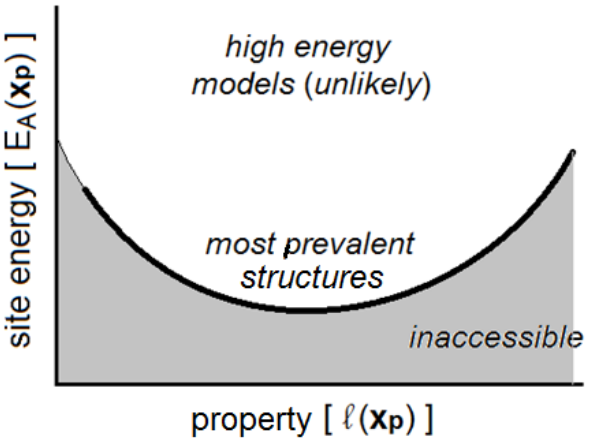
$$H^A_{pp,eff} = H^A_{pp} - H_{pa} H^{-1}_{aa} H_{ap}$$

$$\Delta x_p = -\mathbf{M} g^A_{p,eff} - \Delta \ell \mathbf{e}$$

$$\mathbf{e} = -\frac{H^A_{pp,eff}{}^{-1} \Delta g_{p,eff}}{\Delta g^T_{p,eff} H^A_{pp,eff}{}^{-1} \Delta g_{p,eff}}$$

$$\mathbf{M} = H^A_{pp,eff}{}^{-1} - \frac{H^A_{pp,eff}{}^{-1} \Delta g_{p,eff} \Delta g^T_{p,eff} H^A_{pp,eff}{}^{-1}}{\Delta g^T_{p,eff} H^A_{pp,eff}{}^{-1} \Delta g_{p,eff}}$$





Example: Olefin metathesis by Mo(SiO_2)
subtle variations in the SiO_2 model alter the activation energy for a key step. *Goldsmith, Peters, in prep.*