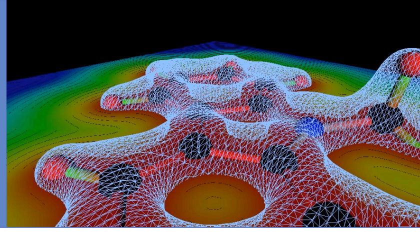
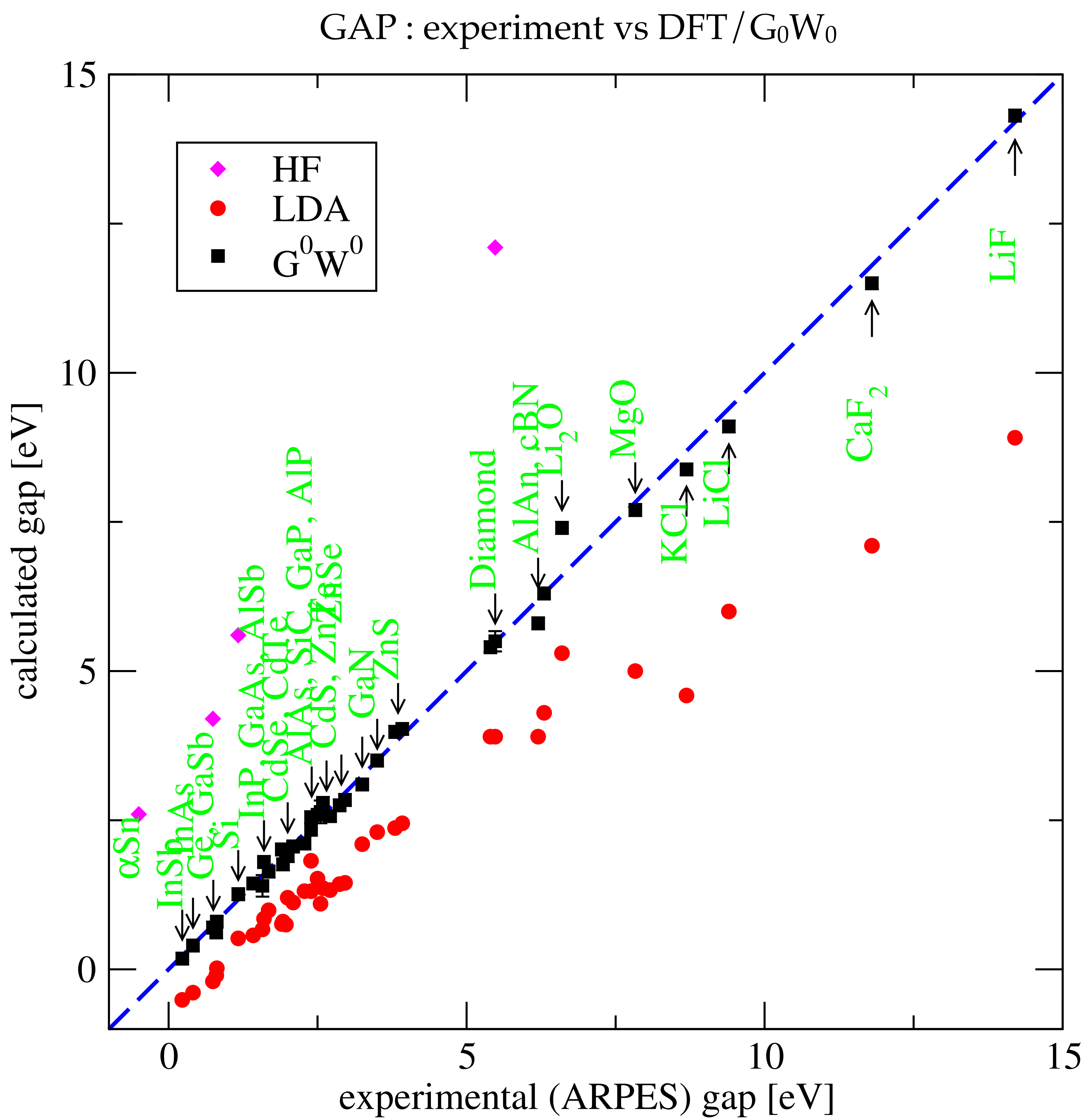
G_0W_0 implementation using Lanczos algorithm and Sternheimer equation

By Jonathan Laflamme Janssen, Nicolas Bérubé, Gabriel Antonius and Michel Côté

Département de physique, Université de Montréal

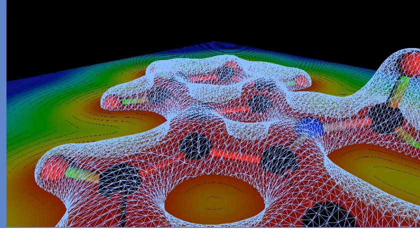
Motivation : gap prediction





S. Faleev, PRL, 2004

Why G_0W_0 computationally expensive?



$$\Sigma = iGW$$

$$W = \epsilon^{-1} v$$

$$\epsilon = 1 - vP$$

$$P = -iGG$$

N_c : number of conduction states

$$G = \sum_{n=1}^{\infty \sim N_c} \frac{|n\rangle\langle n|}{\omega - \varepsilon_n}$$

- $N_c \sim 10\ N_v$ to $100\ N_v$ for ε_i at ±0.05 eV
- inversion of $\epsilon \Rightarrow N^3$ operation (N = basis size)

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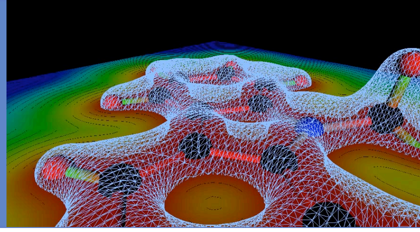

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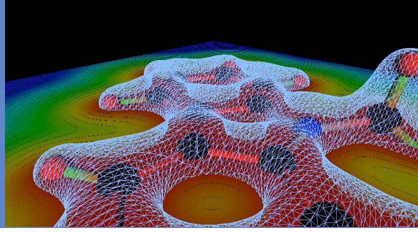

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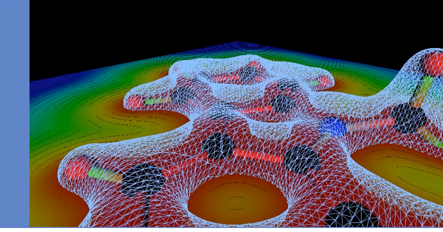
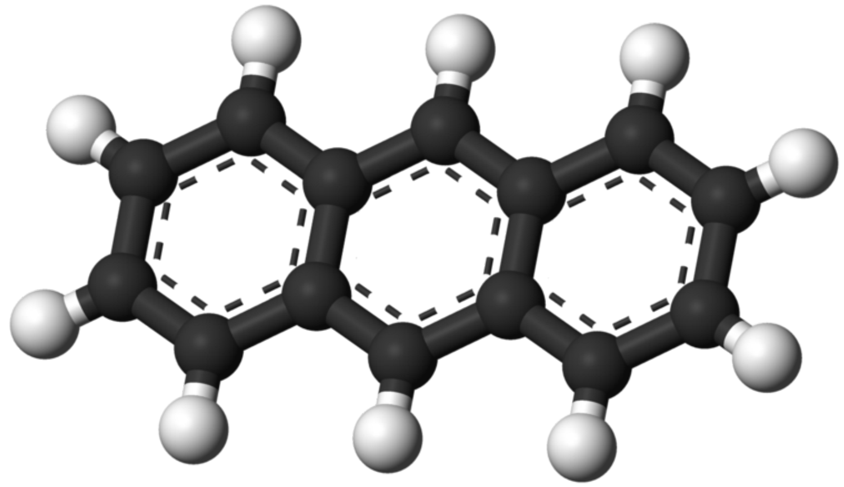
The case of antracene





$N_v = 33$

- $N_c \sim 300$ to 3000 and $N_{basis} \sim 200\,000$
  - ➡ 1 to 10 Gb of RAM usage to store $\{|c\rangle\}$
  - ➡ 100's hours of CPU time to obtain $\{|c\rangle\}$
- ϵ matrix ~ 7000 x 7000 planewaves
  - ➡ 1 Gb of RAM usage to store ϵ
  - ➡ 10's hours of CPU time to ϵ^{-1}

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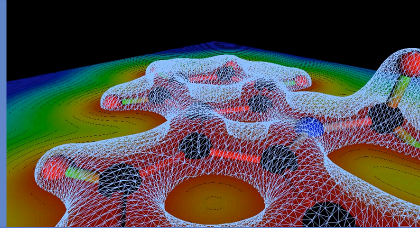

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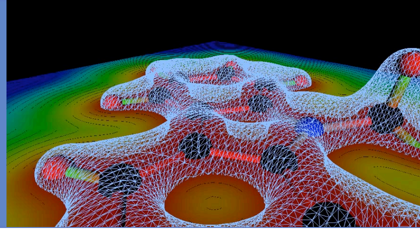

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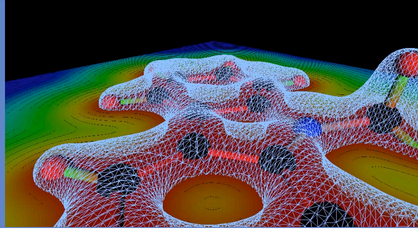

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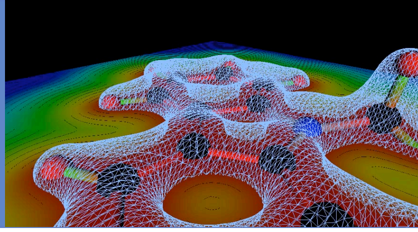

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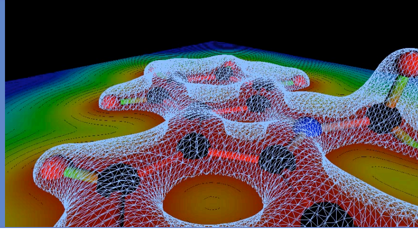
Sternheimer equation



- $$P\left|\psi\right\rangle=\sum_v\left|v\right\rangle\left(\sum_c\left|c\right\rangle\frac{1}{\omega-(\varepsilon_c-\varepsilon_v)}-\frac{1}{\omega+(\varepsilon_c-\varepsilon_v)}\left\langle c\right|\left\langle v\right|\right)\left|\psi\right\rangle$$

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$$\left|\phi_v^-\right\rangle\equiv\sum_c\frac{\left|c\right\rangle\left\langle c\right|}{\omega-(\varepsilon_c-\varepsilon_v)}\left|v\right\rangle\left|\psi\right\rangle=\frac{1}{\omega-H+\varepsilon_v}\mathcal{P}_c\left|v\right\rangle\left|\psi\right\rangle$$

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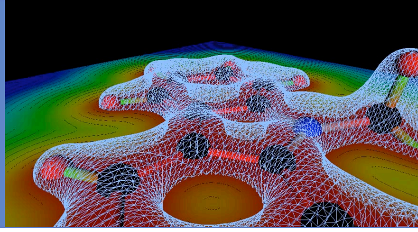

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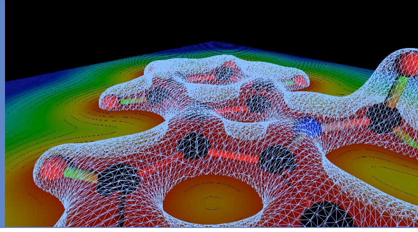

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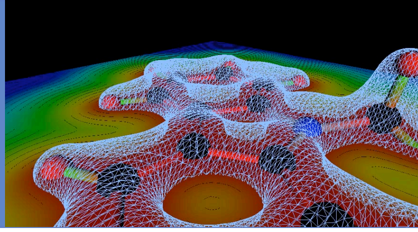

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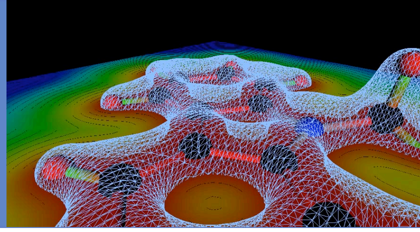

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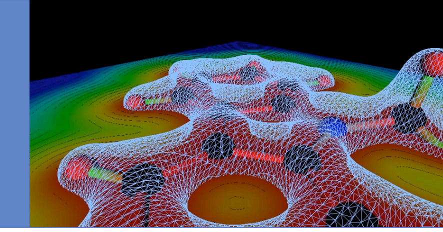

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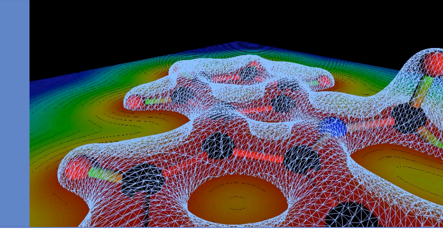

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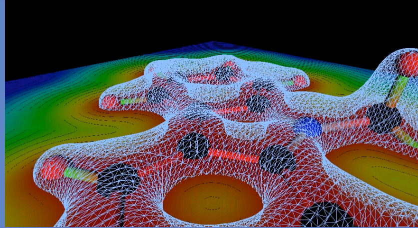
$\cancel{\sum_c}$ $\longrightarrow$ Solving $\boxed{A|x\rangle = |b\rangle}$

$2)\ W = \epsilon^{-1} v$

Lanczos algorithm



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- Lanczos algorithm...
  - builds a basis spanning the same subspace as $\left\{ (vP)^k |\psi\rangle \right\}$
  - where (vP) is tridiagonal
  - at the same cost as using the power serie expansion

- In Lanczos basis $\{|q_k\rangle\}$: $\sum_{k=0}^{+\infty} (vP)^k |\psi\rangle = \sum_{k=0}^{+\infty} T^k |q_1\rangle$

$$= (1-T)^{-1} |q_1\rangle$$

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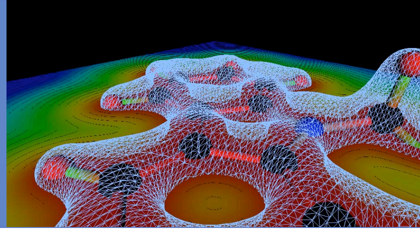

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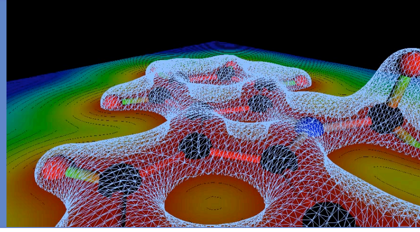
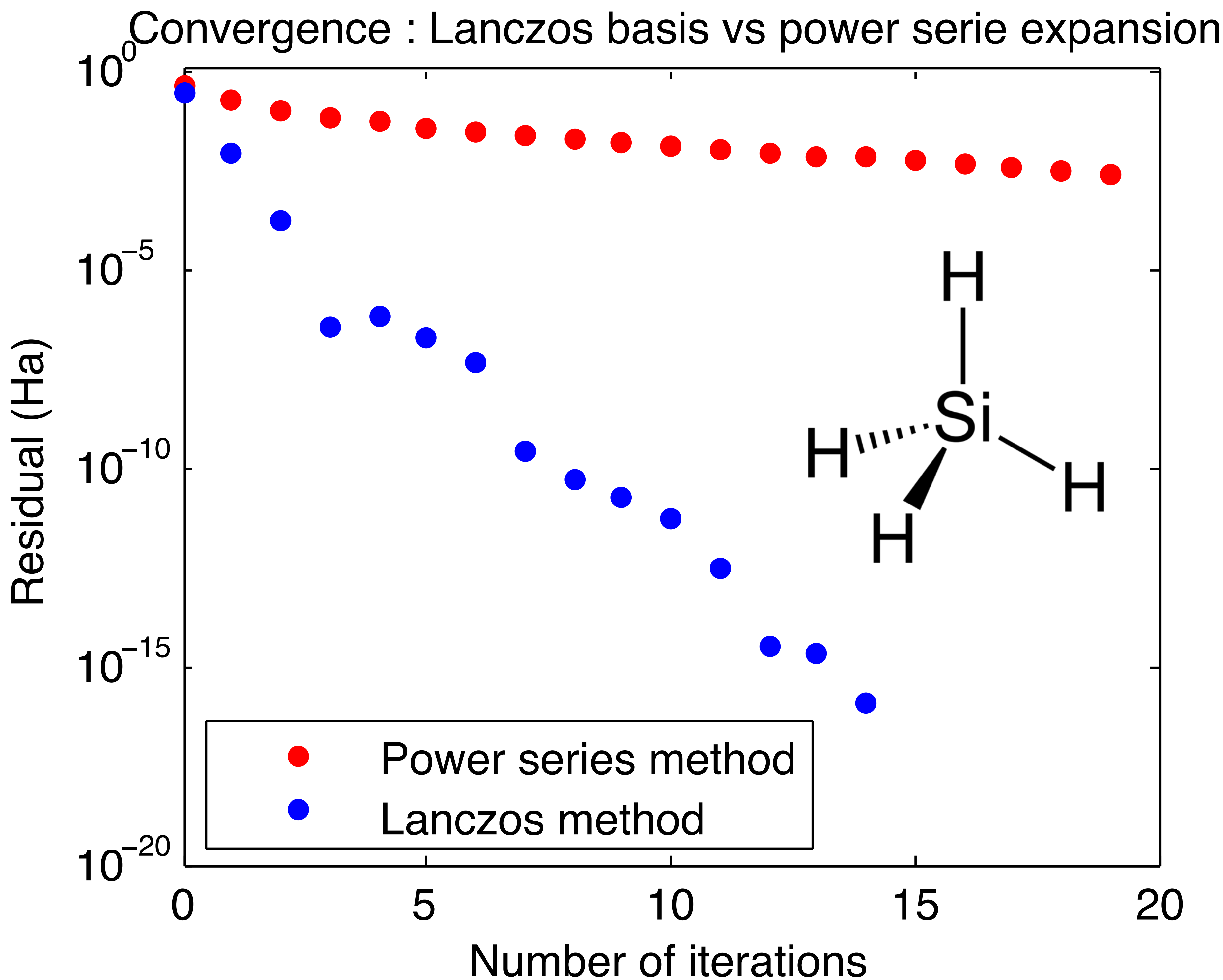
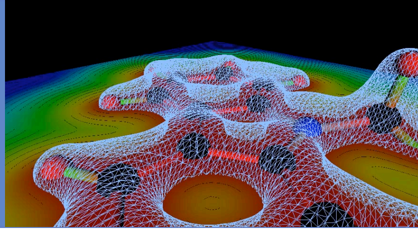


Calculation of screened exchange for HOMO of silane



Sternheimer's equation



- Same idea as for *P* :

$$\cancel{\sum_c} \longrightarrow \quad \text{Solving } \boxed{A|x\rangle = |b\rangle}$$

- But requires $\{|q_k\rangle\}$

$$|g_k\rangle = \sum_n \frac{|n\rangle\langle n|}{\omega' - (\varepsilon_n - \varepsilon_i)} |i\rangle |q_k\rangle$$

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$$\langle i|\Sigma(\varepsilon_i)|i\rangle = \frac{i}{2\pi}\int_{-\infty}^{+\infty} d\omega' \sum_{k,k'} (1-T)^{-1}_{k,k'} \langle (vq_{k'})i|g_k\rangle$$

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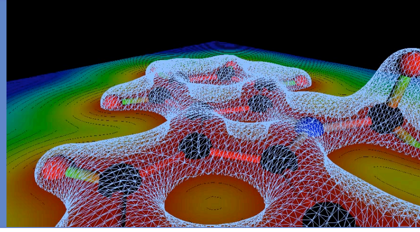

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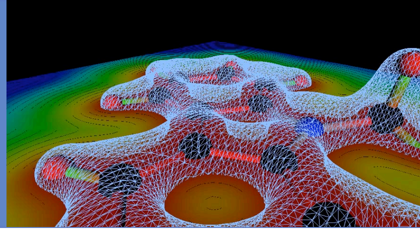

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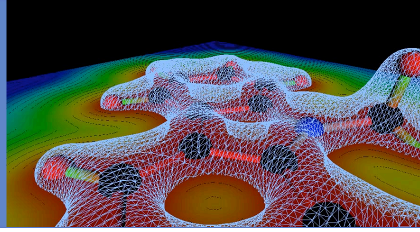

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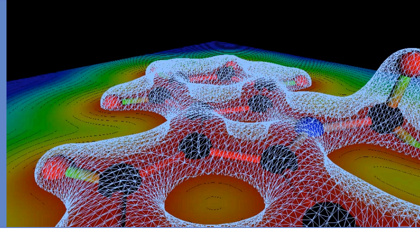

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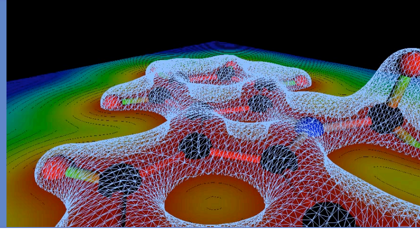
Conclusion



- Bottleneck assessed :
  - no knowledge of conduction states required
  - no inversion of ϵ in cumbersome basis

- Implementation under way

Thank you!

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