"G0W0 implementation using Lanczos algorithm and Sternheimer equation"

Laflamme Janssen, Jonathan ; Bérubé, Nicolas ; Antonius, Gabriel

Abstract

The G0W0 approach is an accurate method to give a physical meaning to the eigenvalues obtained in adensity-functional theory (DFT) calculation.However, the calculation of such corrections with plane wave codes is currently prohibitive for systems with more than a few hundreds of electrons. What limits calculations to this system size is the need in current implementations to invert the dielectric matrix and the need to carry out summations over conduction bands. This talk presents a strategy to avoid both of these bottlenecks. In traditional plane wave implementations of G0W0, the dielectric matrix is expressed in a plane wave basis, which needs to be relatively big to properly describe the matrix. Here, we will explain how a Lanczos basis can be generated to substantially reduce the size of the matrix. Also, the number of conduction bands needed to reach convergence in the summations is usually an order of magnitude larger than the number of valence bands. Here, the calculation of t...

Document type : *Communication à un colloque (Conference Paper)*

Référence bibliographique

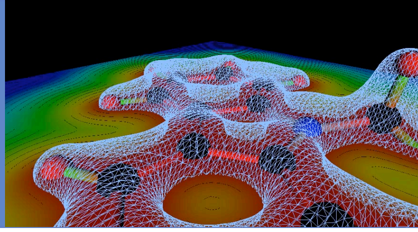
Laflamme Janssen, Jonathan ; Bérubé, Nicolas ; Antonius, Gabriel. *G0W0 implementation using Lanczos algorithm and Sternheimer equation.*APS March Meeting 2012 (Boston, Massachusetts, USA, du 27/02/2012 au 02/03/2012).

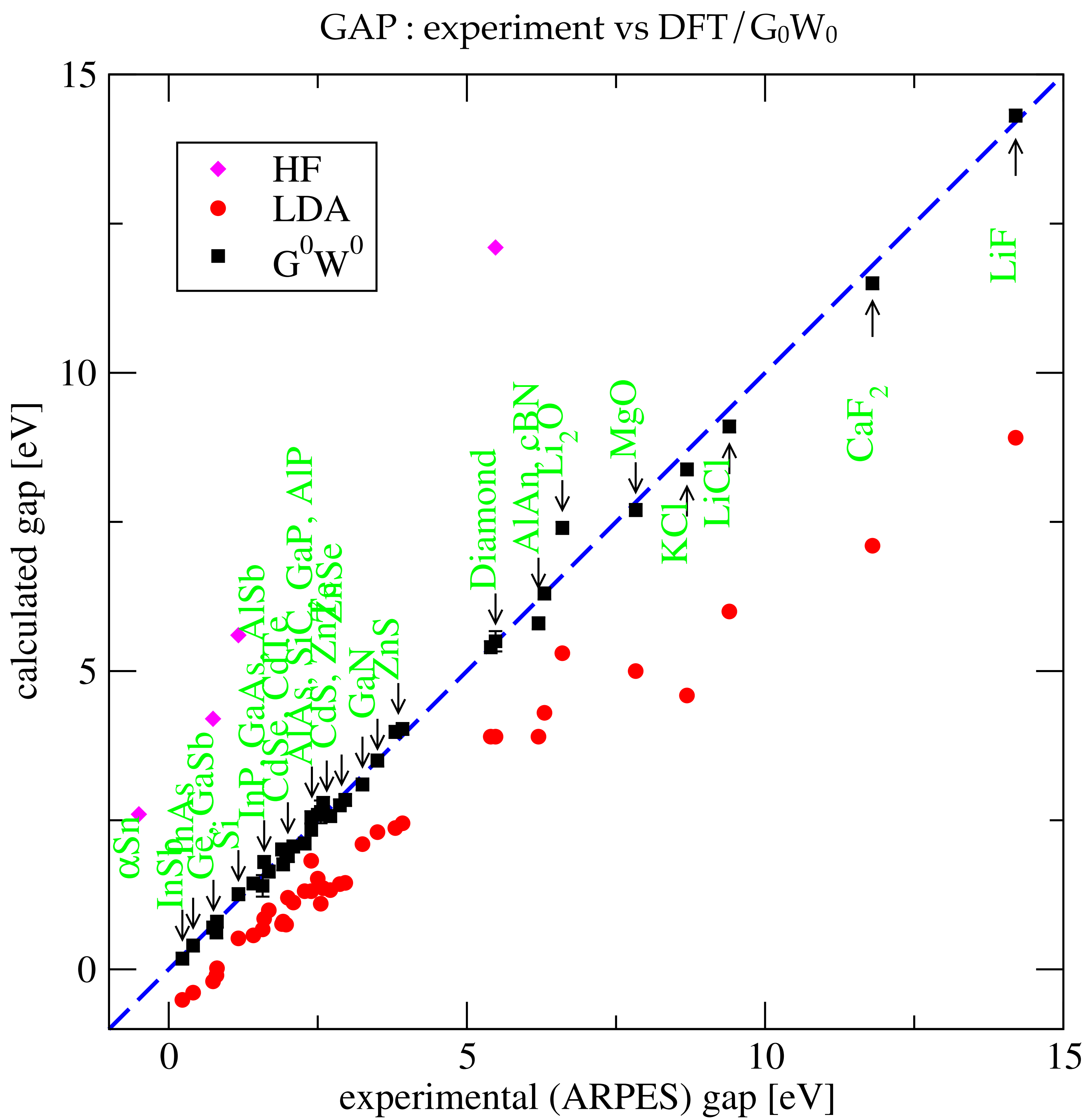
G_0W_0 implementation using Lanczos algorithm and Sternheimer equation

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

Département de physique, Université de Montréal

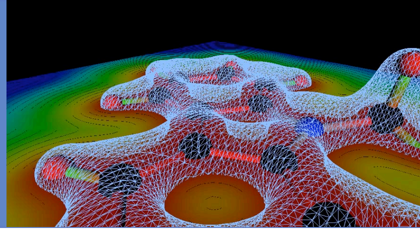
Motivation : gap prediction





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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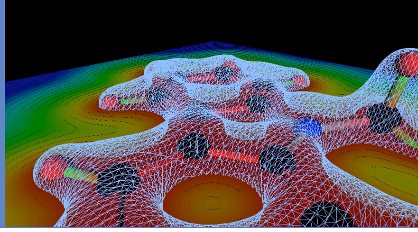

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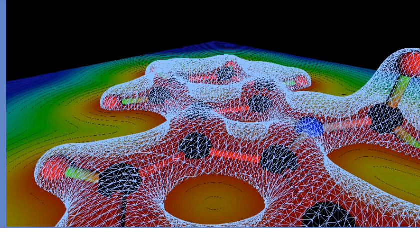

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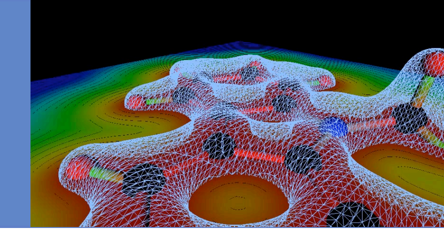

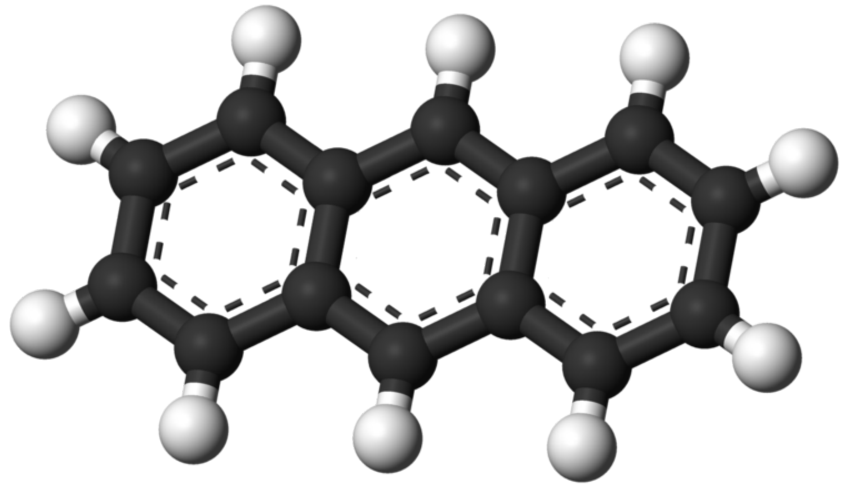

$N_v = 33$

- N_c ~ 300 to 3000 and N_{basis} ~ 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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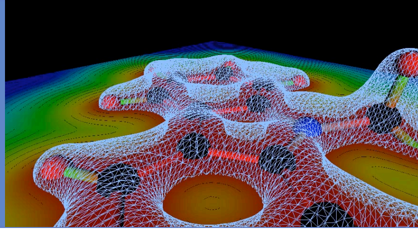

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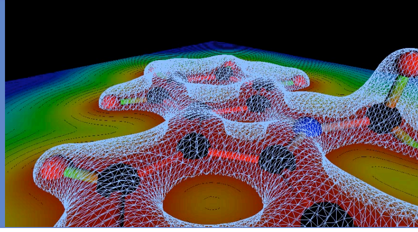

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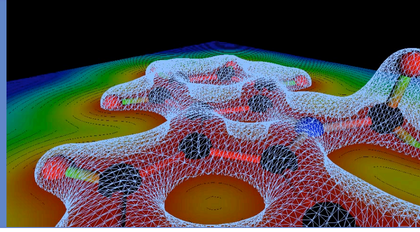

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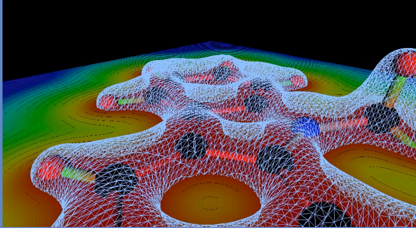

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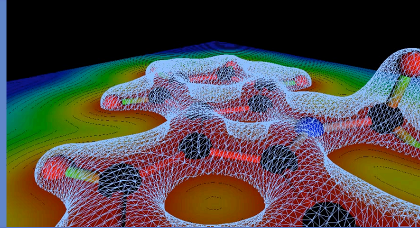
Sternheimer equation



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

- We define :

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

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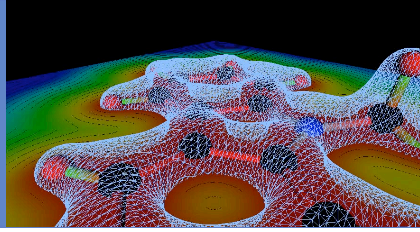
$$\left(H-\varepsilon_v-\omega\right)\left|\phi_v^-\right\rangle = -\mathcal{P}_c\left|v\right\rangle\left|\psi\right\rangle$$ Sternheimer equation

Sternheimer equation



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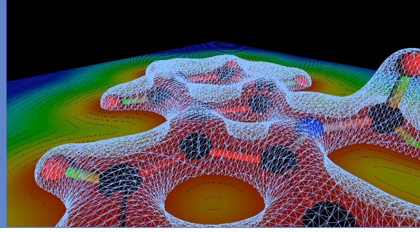

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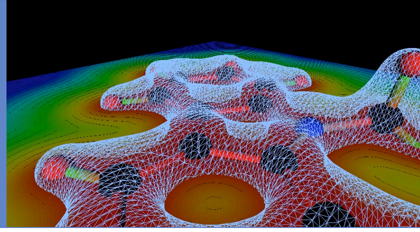

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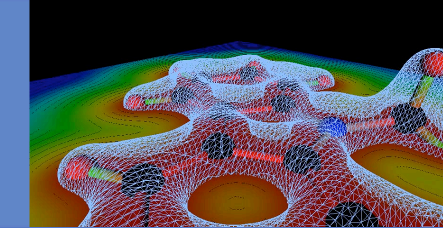

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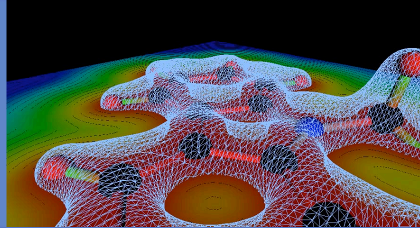

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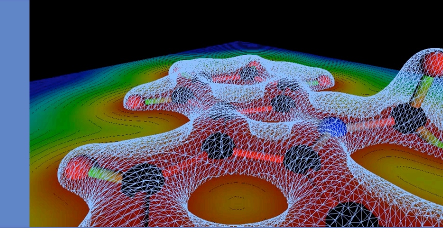

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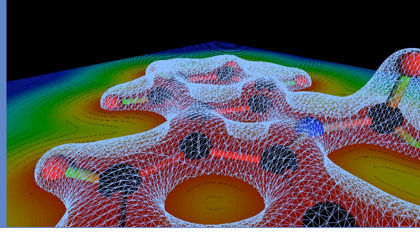

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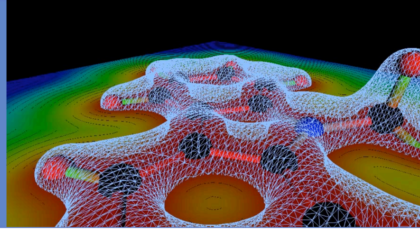
$\cancel{\sum_c} \longrightarrow$ Solving $\boxed{A|x\rangle = |b\rangle}$

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

Lanczos algorithm



- $$\epsilon^{-1}|\psi\rangle = (1 - vP)^{-1}|\psi\rangle = \sum_{k=0}^{+\infty}(vP)^k|\psi\rangle$$

- 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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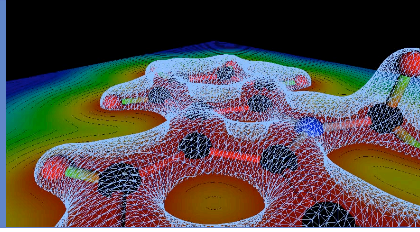

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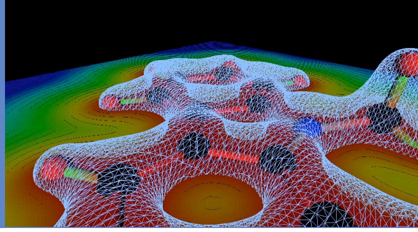
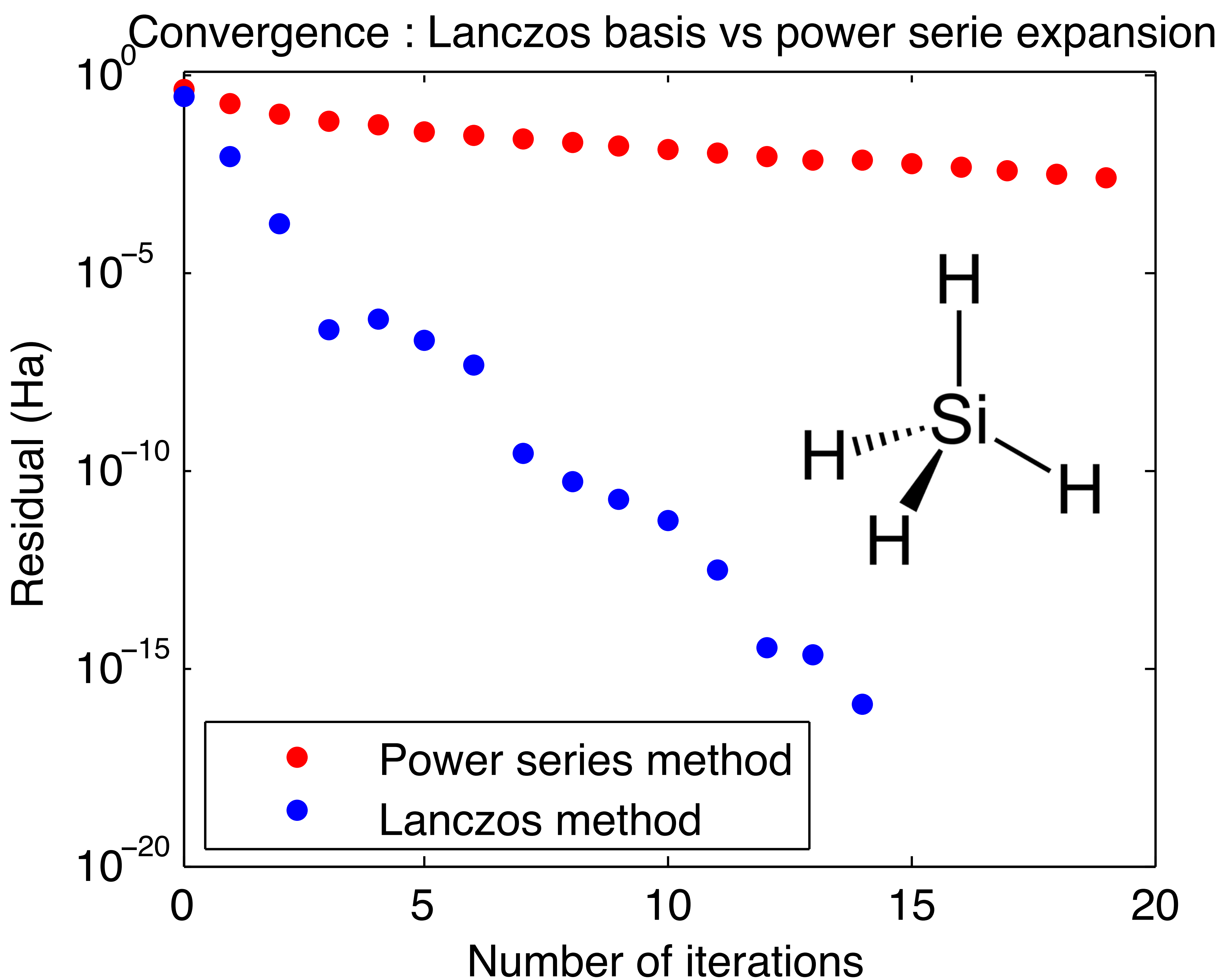


Calculation of screened exchange for HOMO of silane



Sternheimer's equation

- Same idea as for *P* :

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

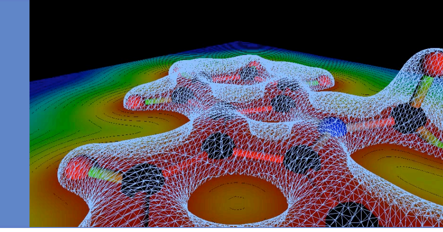
- But requires $\{|q_k\rangle\}$

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

$$\left(H - \varepsilon_i - \omega'\right)|g_k\rangle = -1|q_k i\rangle$$ Sternheimer equation

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

3) $\Sigma = iGW$ Sternheimer's equation



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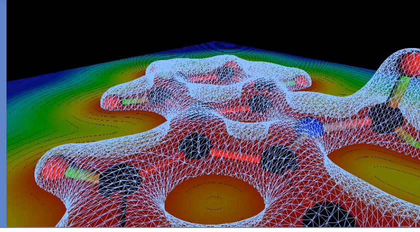

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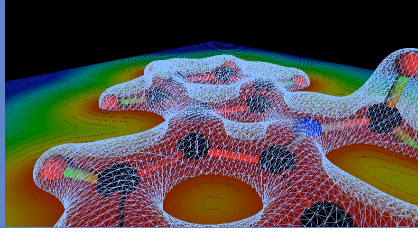

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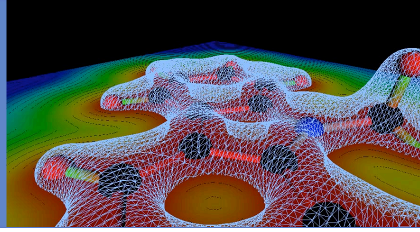

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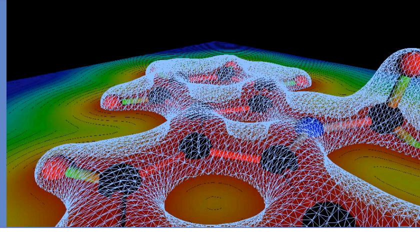
Conclusion



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

Thank you!

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