Accurate effective masses from first principles

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UCL Université catholique de Louvain

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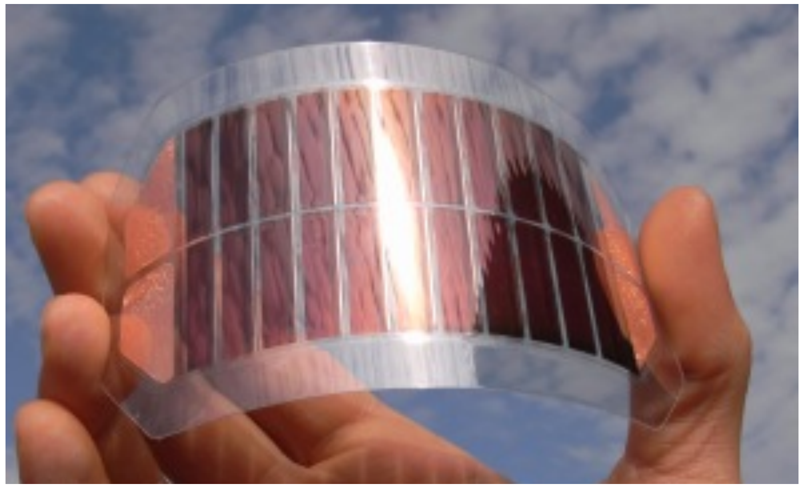

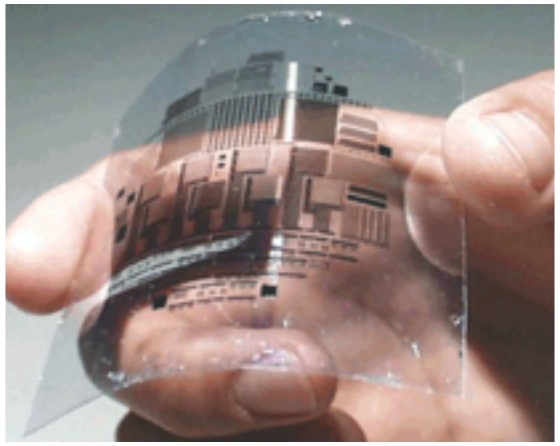

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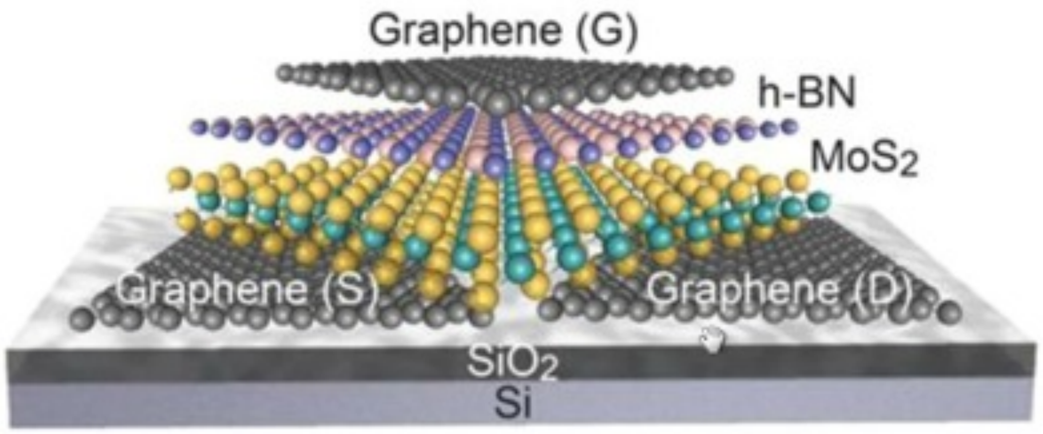

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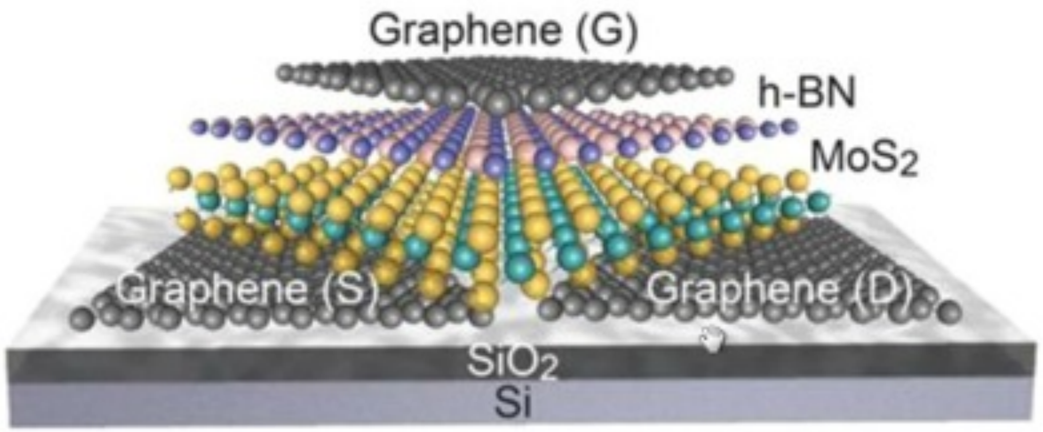

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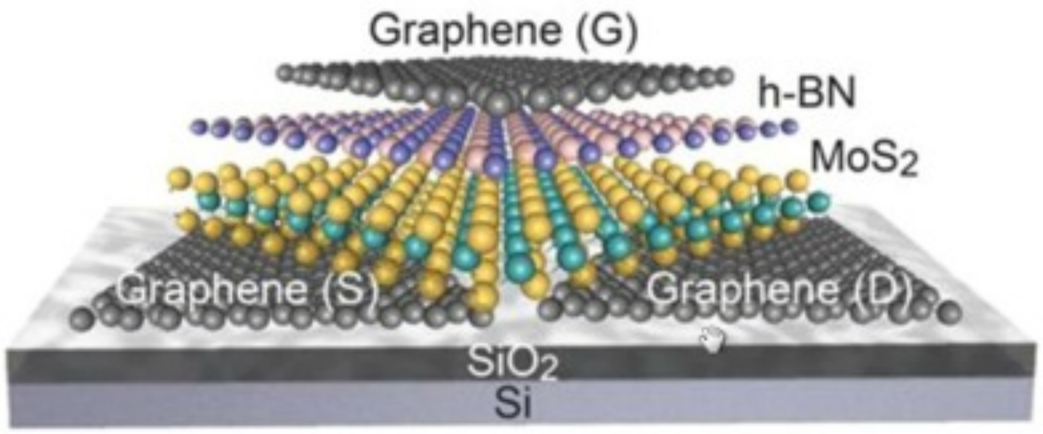

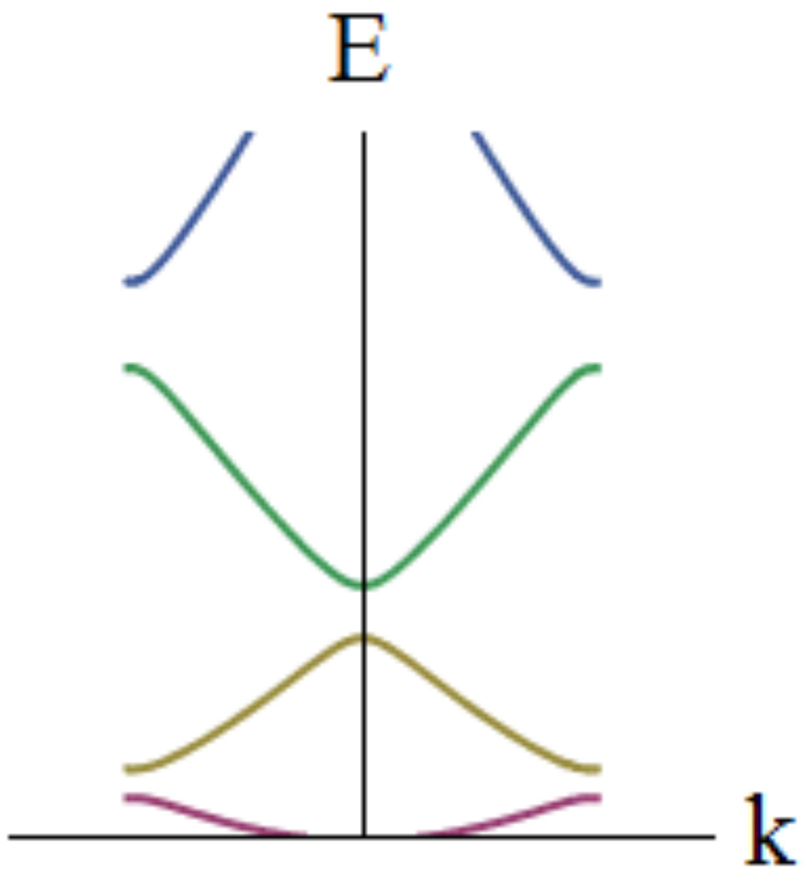

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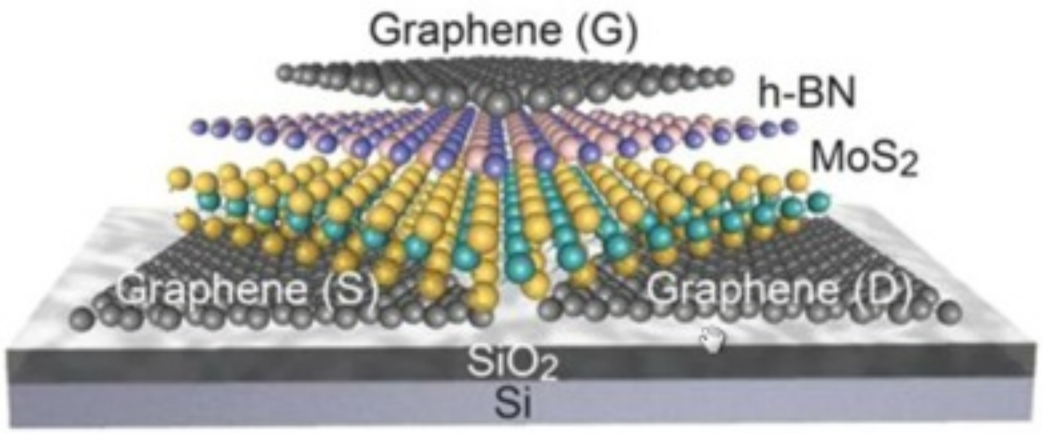

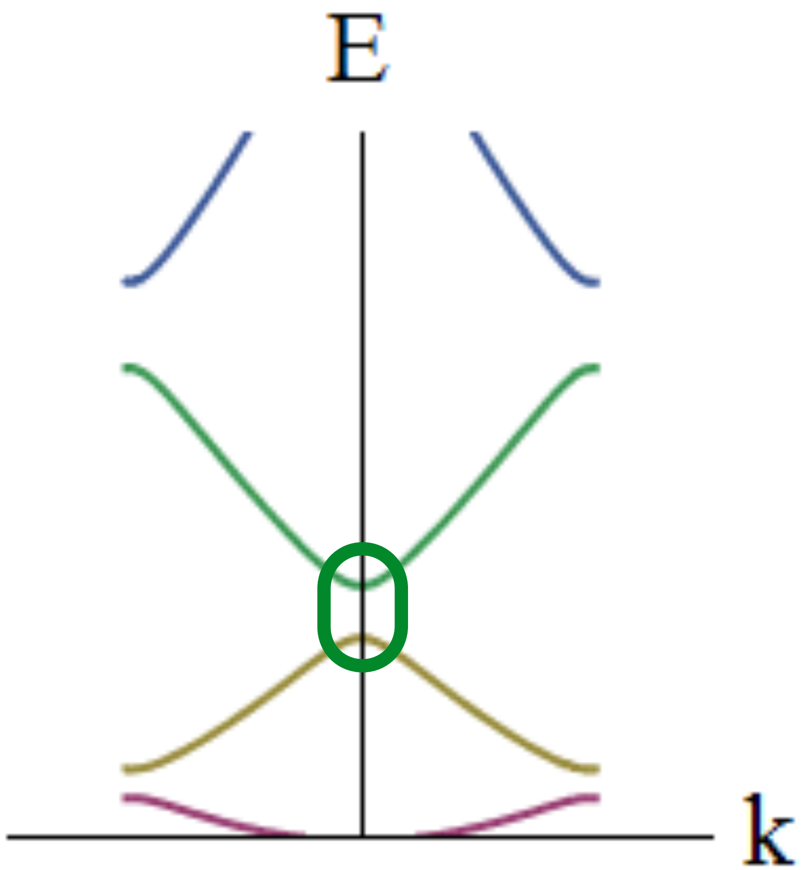

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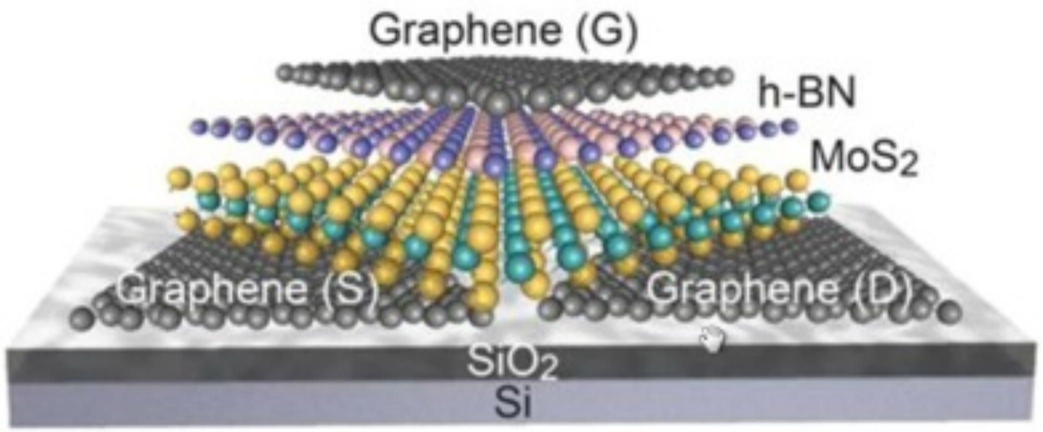

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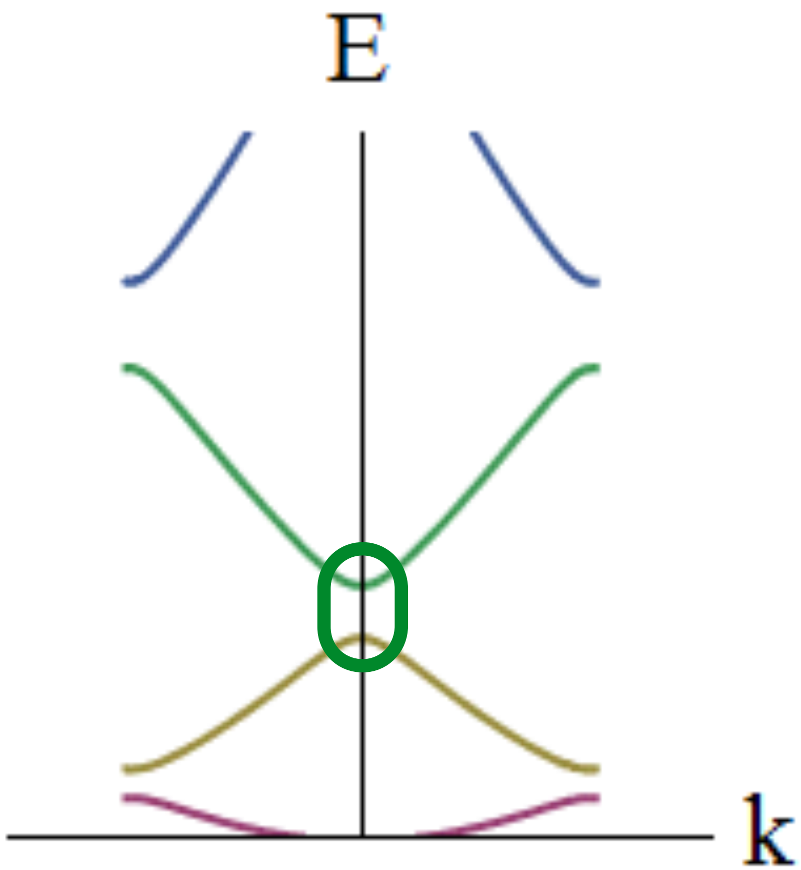

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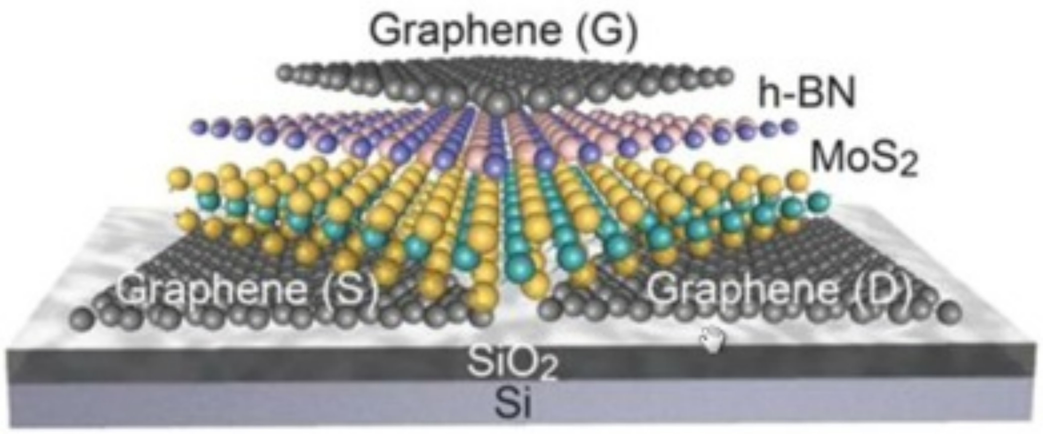

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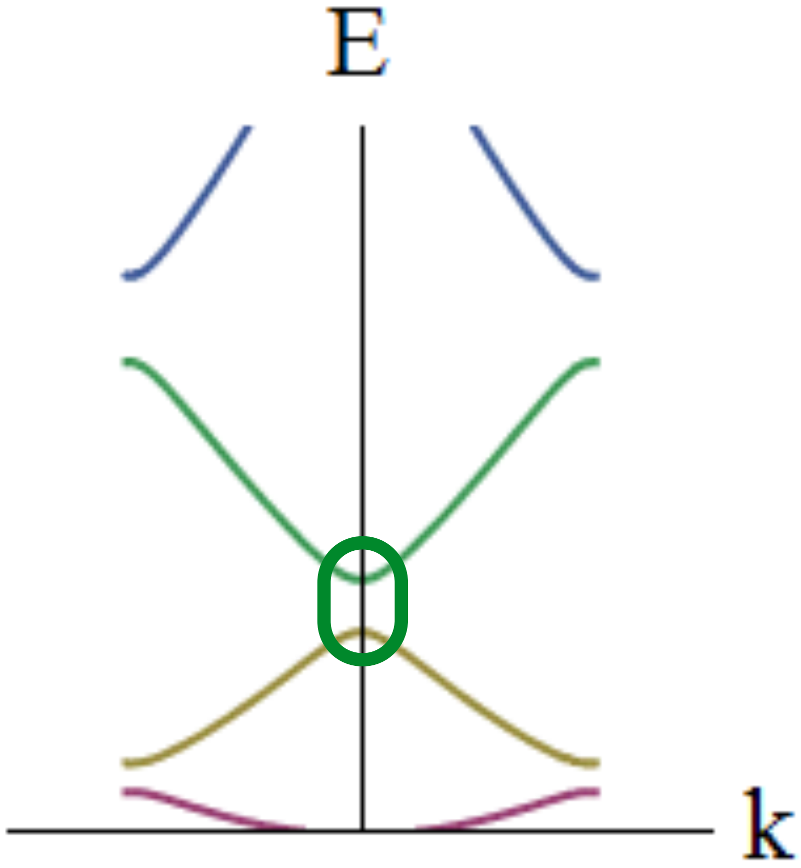

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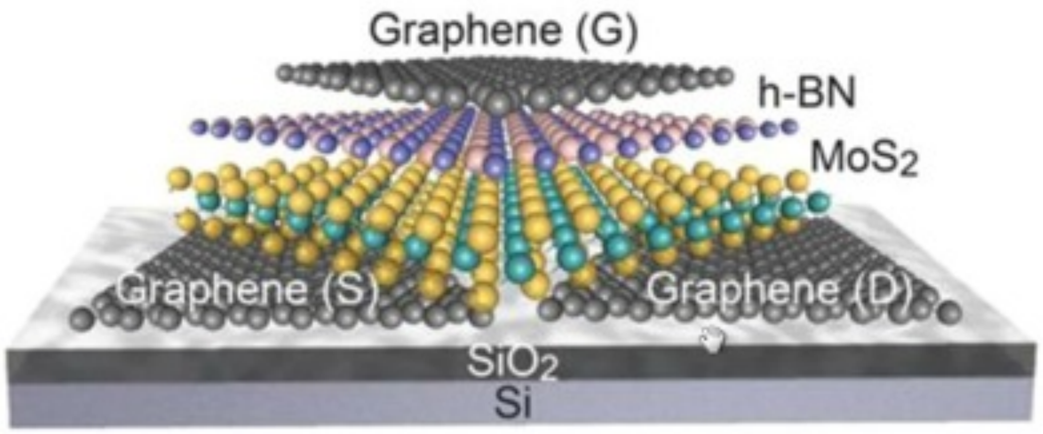

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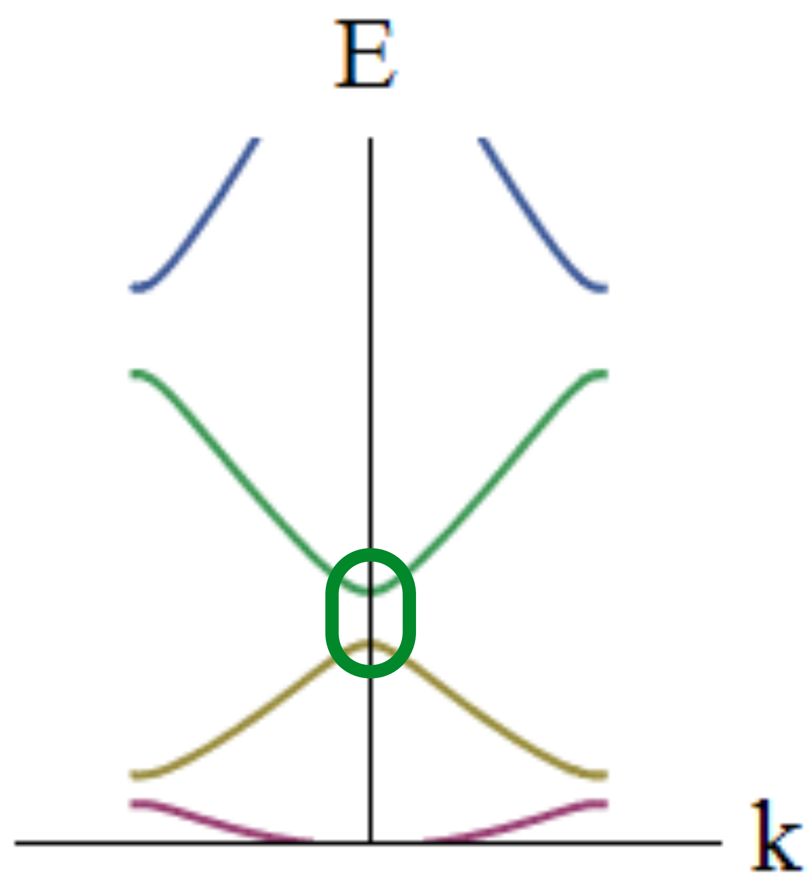

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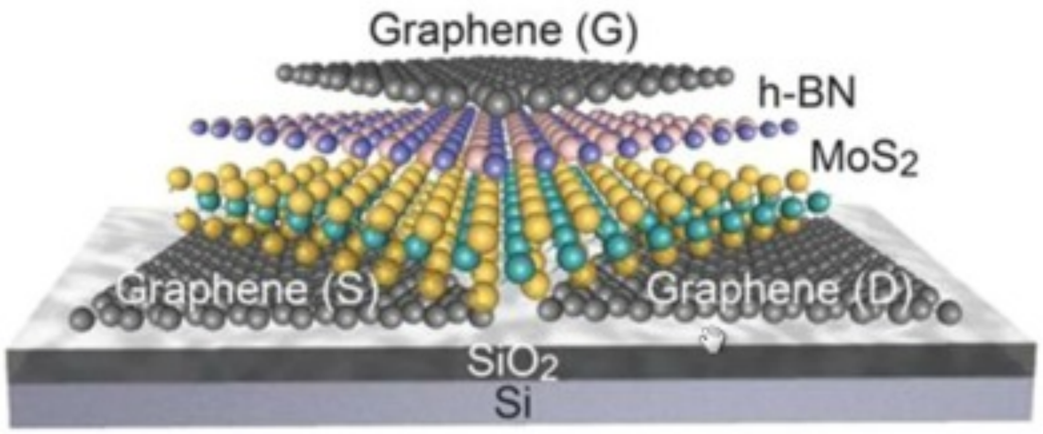

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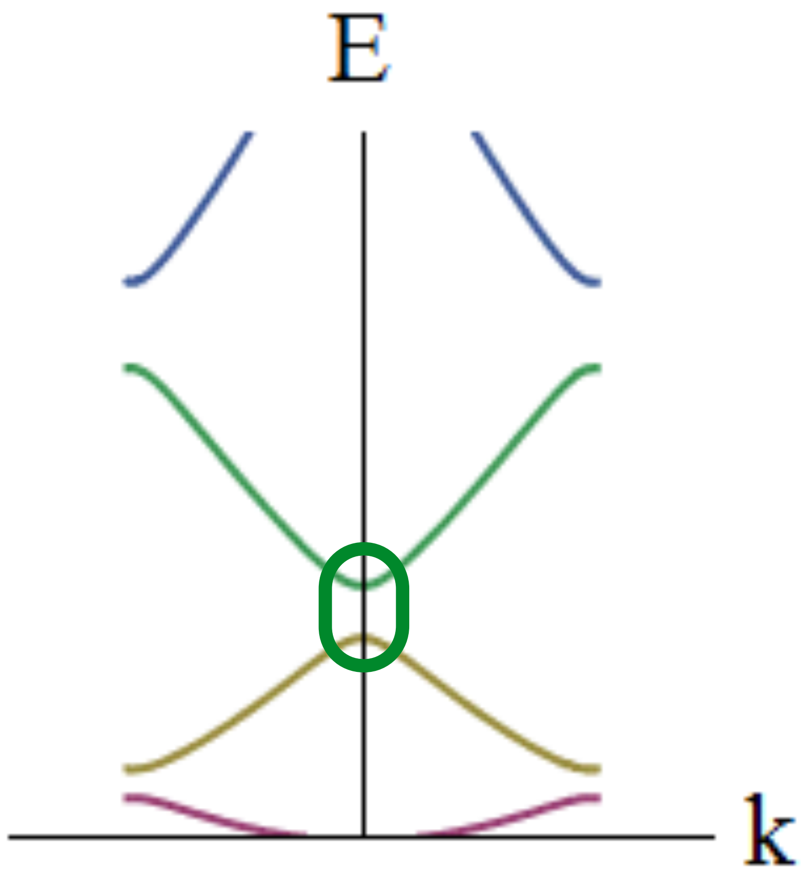

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Derivatives of $\hat{H}$ up to 2nd order

DFPT

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0.000	1.161	-0.000
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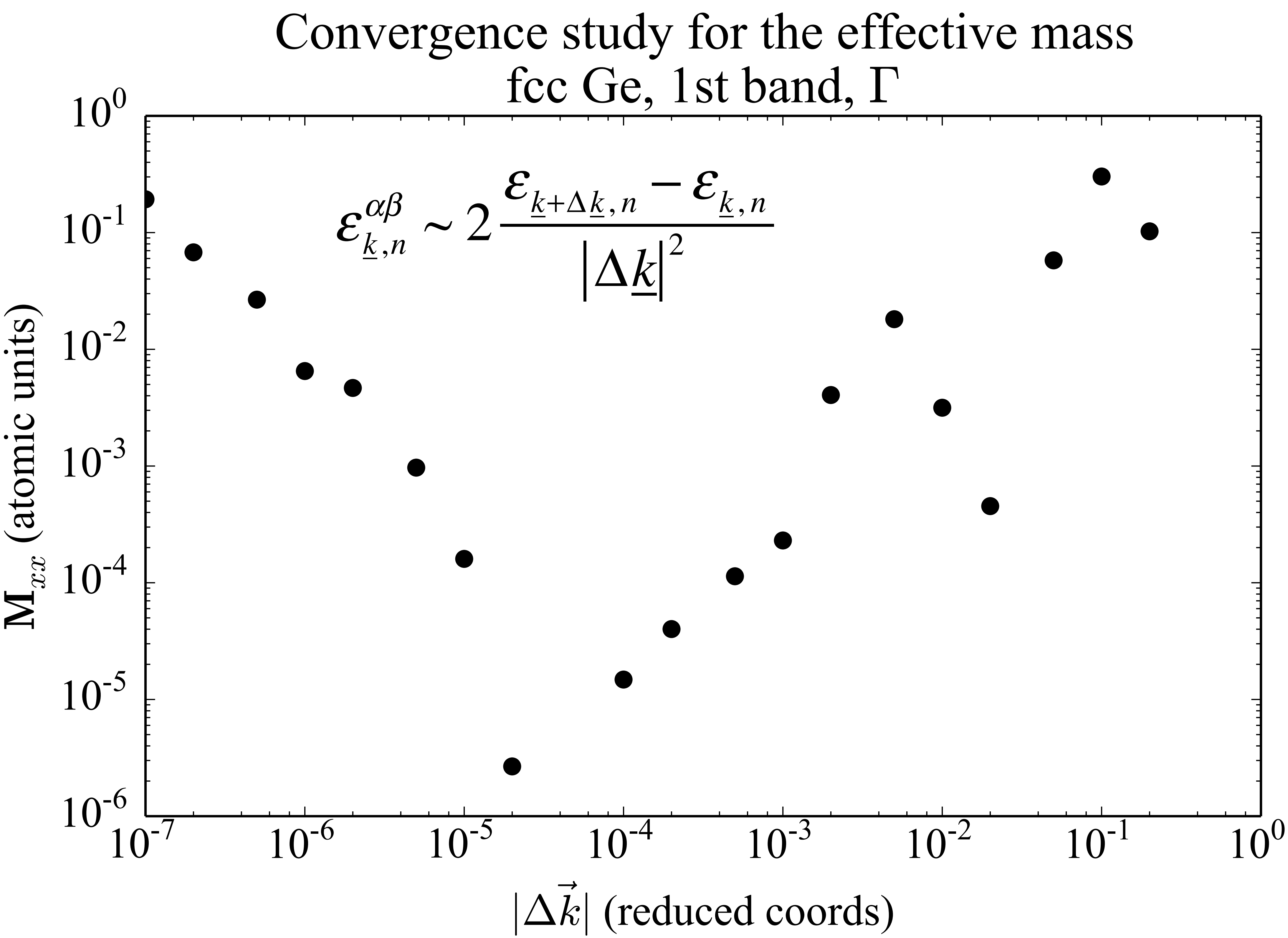
$$\varepsilon_{\underline{k},n}^{\alpha\beta} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$$

Numerical noise : finite differences



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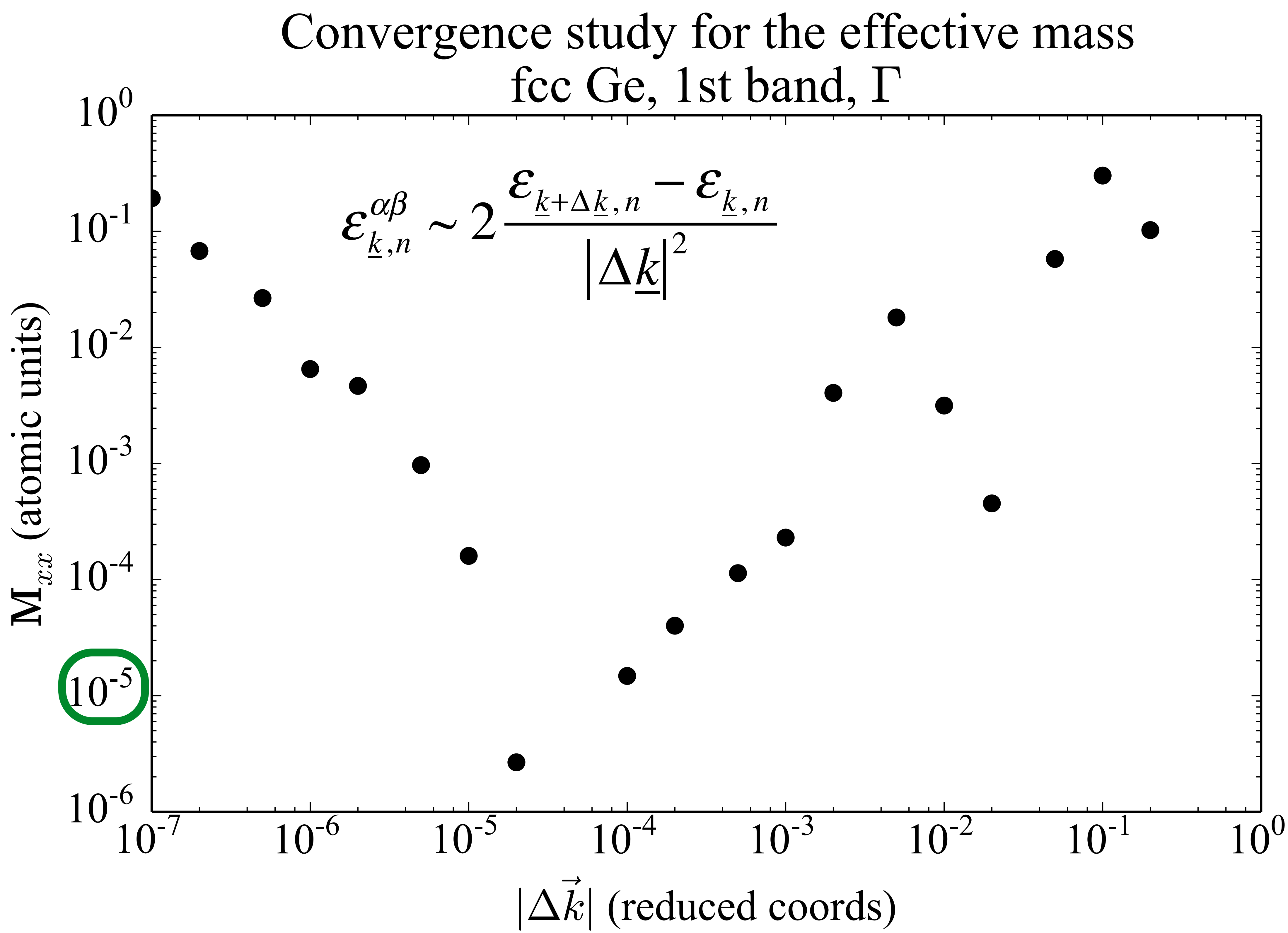

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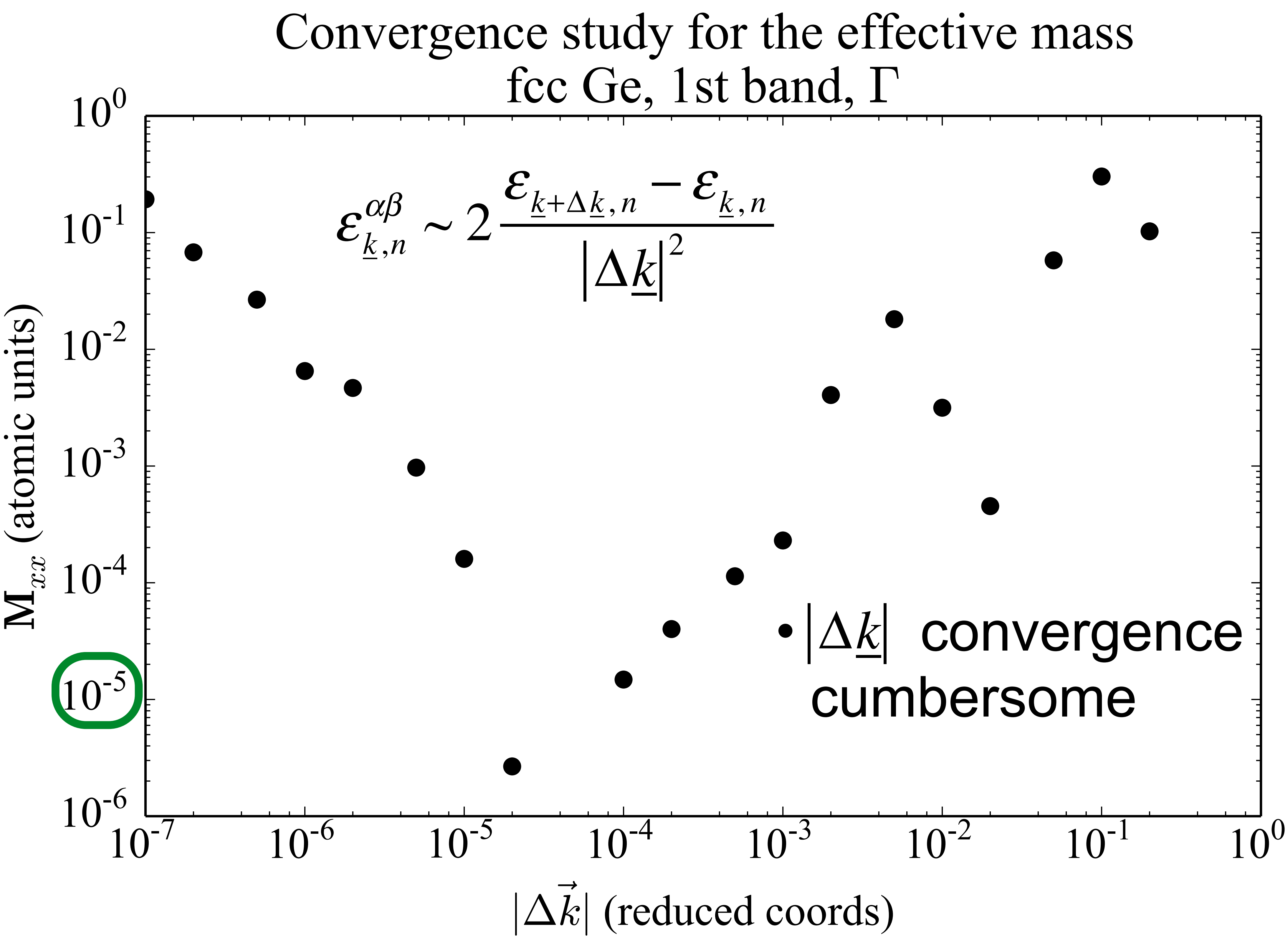

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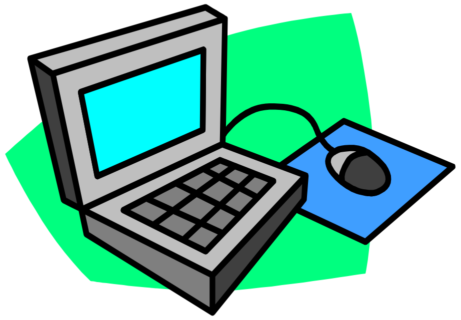

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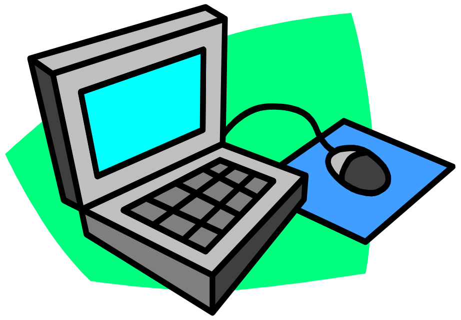

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ETSF

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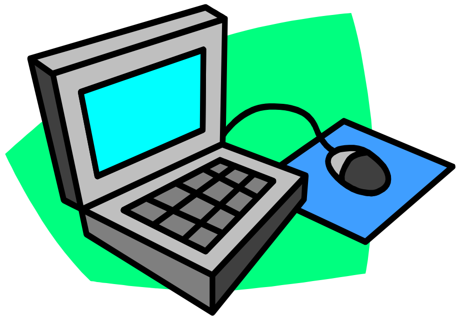
Thank you!



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Future directions

Future directions

- Correction factor for e-e interactions

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$$\frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}} = \frac{\partial^2 \varepsilon^{\mathrm{DFT}} \big/ \partial k^2}{\partial^2 \varepsilon^{\mathrm{G_0W_0}} \big/ \partial k^2} = \frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}}$$

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$$\partial \varepsilon^{\mathrm{G_0W_0}} = \partial \varepsilon^{\mathrm{DFT}} + \frac{\partial \left\langle \hat{\Sigma}(\omega) \right\rangle}{\partial k} \delta k + \frac{\partial \left\langle \hat{\Sigma}(\omega) \right\rangle}{\partial \omega} \delta \varepsilon^{\mathrm{G_0W_0}}$$

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Oshikiri et al. PRB **66** 125204 (2002)

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<0.02% M in AlAs

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$$\frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}} = 1 - \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} = \frac{1}{Z}$$

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$$\partial\varepsilon^{\mathrm{G_0W_0}}=\partial\varepsilon^{\mathrm{DFT}}+\cancel{\frac{\partial\left\langle\hat{\Sigma}(\omega)\right\rangle}{\partial k}}\delta k+\boxed{\frac{\partial\left\langle\hat{\Sigma}(\omega)\right\rangle}{\partial\omega}\delta\varepsilon^{\mathrm{G_0W_0}}}$$

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$$\frac{\partial\varepsilon^{\mathrm{DFT}}}{\partial\varepsilon^{\mathrm{G_0W_0}}}=1-\frac{\partial\left\langle\hat{\Sigma}(\omega)\right\rangle}{\partial\omega}=\frac{1}{Z}=\frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}}$$

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- How general is this apprx?