2023 Virtual School on Many-Body Calculations using **EPW** and **BerkeleyGW**

5-9 June 2023

NSF

U.S. DEPARTMENT OF ENERGY

TACC
TEXAS ADVANCED COMPUTING CENTER

Lecture Wed.1

Theory of polarons

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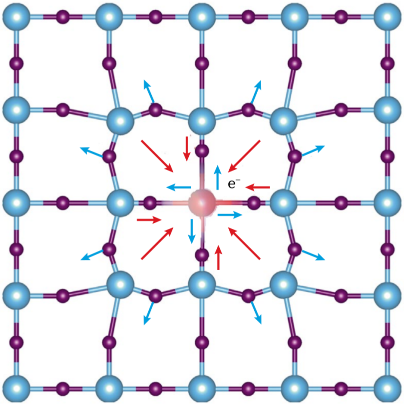
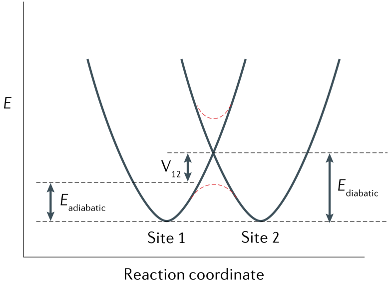
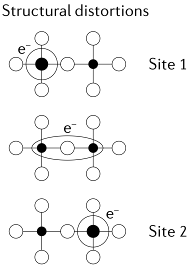
Oden Institute & Department of Physics

The University of Texas at Austin

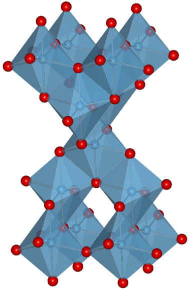
- Introduction to the polaron concept
- Photoemission spectra
- DFT calculations of polarons
- Landau-Pekar theory
- *Ab initio* polaron equations
- Examples of polarons
- Many-body theory of polarons



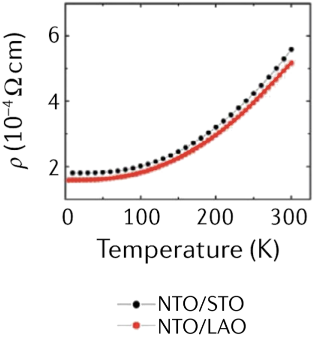




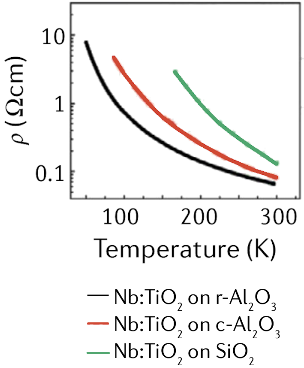
Figures from Franchini et al, Nat. Rev. Mater. 2021, 10.1038/s41578-021-00289-w

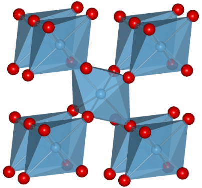


Anatase TiO_2



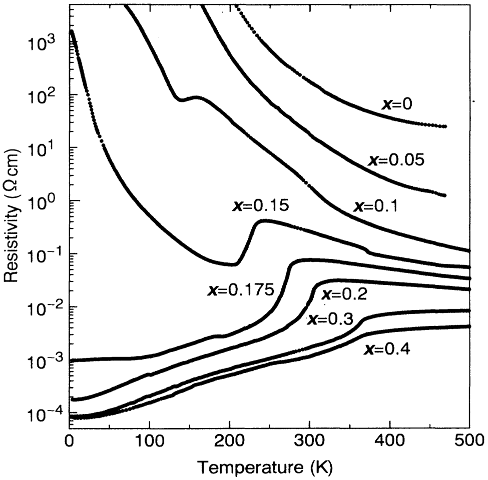
Rutile TiO_2





Hall mobility data from Zhang et al, J. Appl. Phys. 102, 013701 (2007)

Transport signatures of polarons



$La_{1-x}Sr_xMnO_3$

Figure from Urushibara, Moritomo, Arima, Asamitsu, Kido, Tokura, Phys. Rev. B 51, 14103 (1995)

Angle-resolved photoelectron spectroscopy (ARPES)

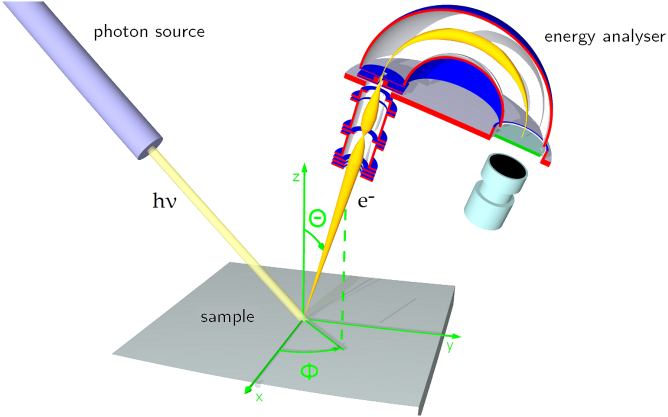


Figure from commons.wikimedia.org/wiki/File:ARPESgeneral.png

Phonon satellites in anatase TiO_2

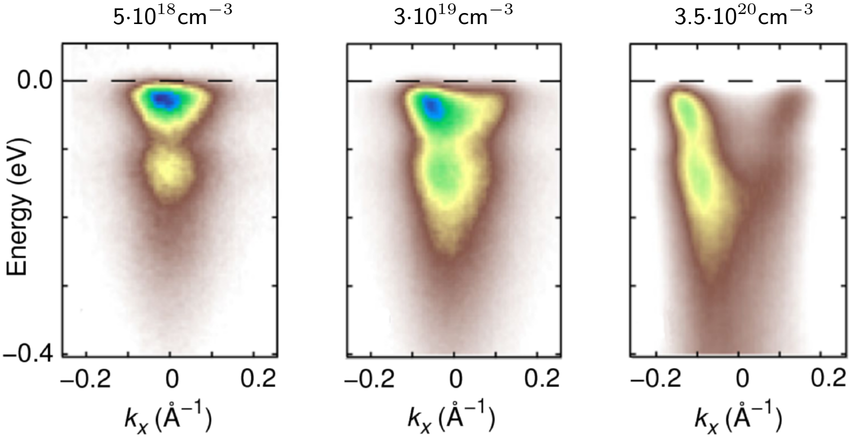


Figure from Moser et al, Phys. Rev. Lett. 110, 196403 (2013)

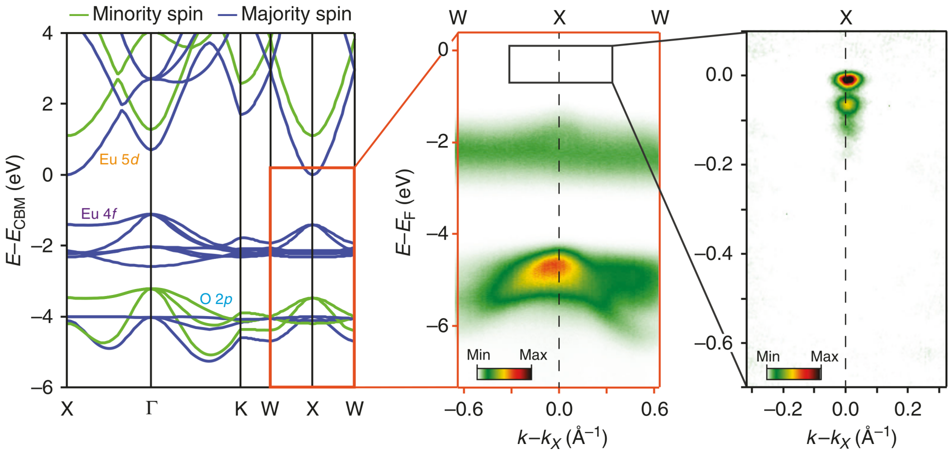
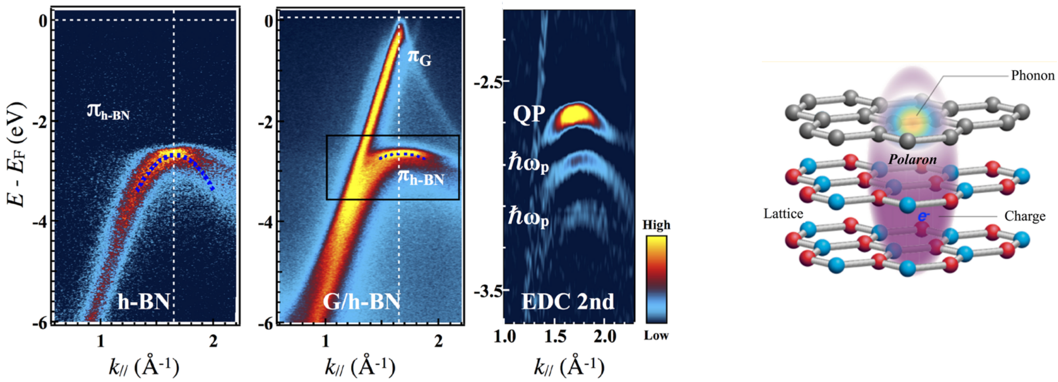


Figure from Riley et al, Nat. Commun. 9, 2305 (2018)



Figures from Chen et al, Nano Lett. 18, 1082 (2018)

Polaron satellites (aka phonon sidebands)

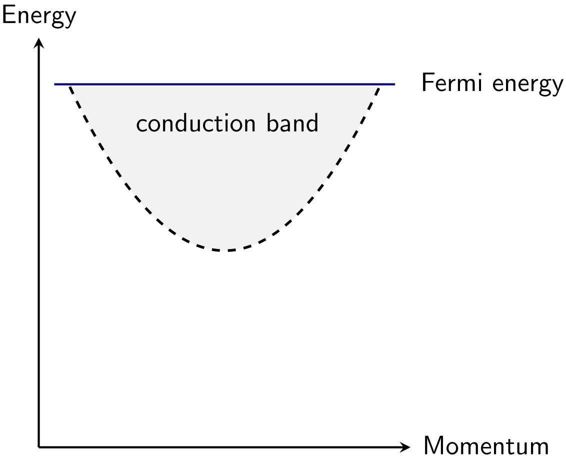


Figure adapted from Kandolf et al, Phys. Rev. B 105, 085148 (2022)

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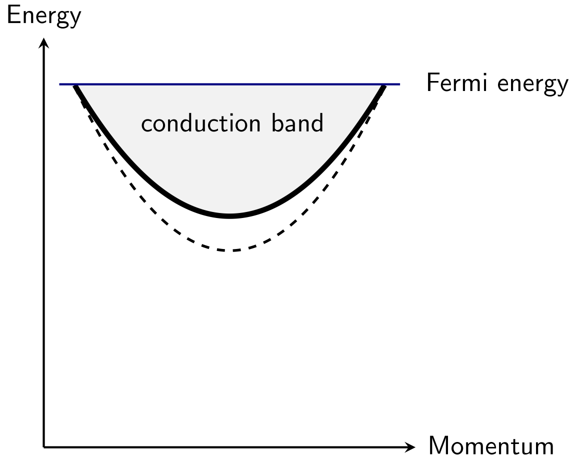

Figure adapted from Kandolf et al, Phys. Rev. B 105, 085148 (2022)

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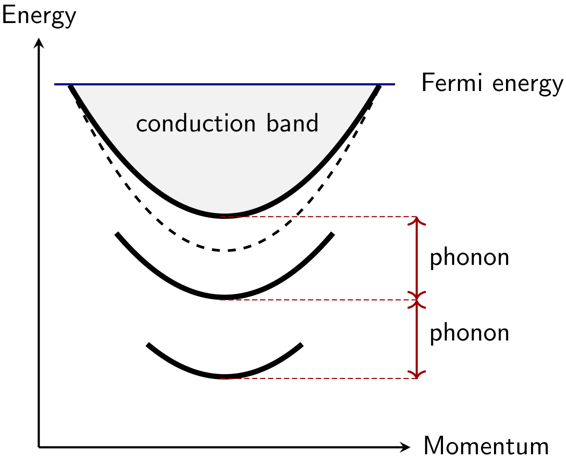


Figure adapted from Kandolf et al, Phys. Rev. B 105, 085148 (2022)

Electron mass enhancement vs. phonon satellites in ARPES

$\hbar\omega_{\rm ph} \ll \varepsilon_{\rm F}$: Mass enhancement

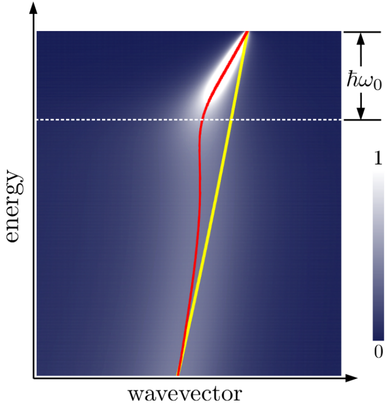


Figure from FG, Rev. Mod. Phys. 89, 015003 (2017)

Electron mass enhancement vs. phonon satellites in ARPES

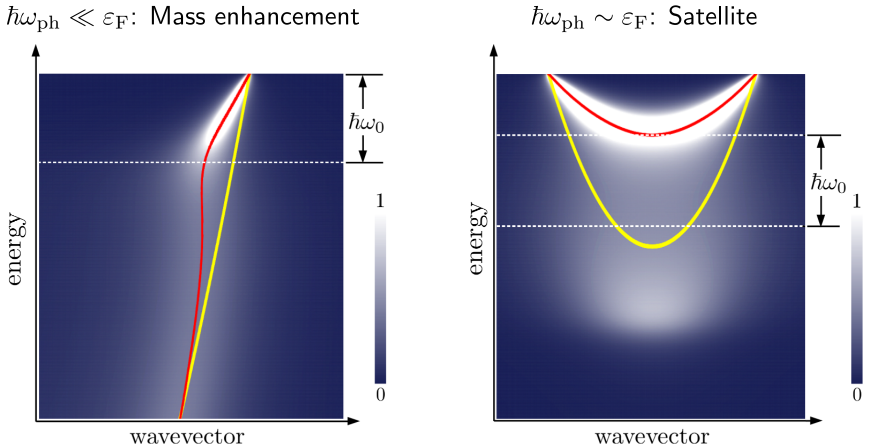


Figure from FG, Rev. Mod. Phys. 89, 015003 (2017)

Calculated vs. measured spectral function: EuO

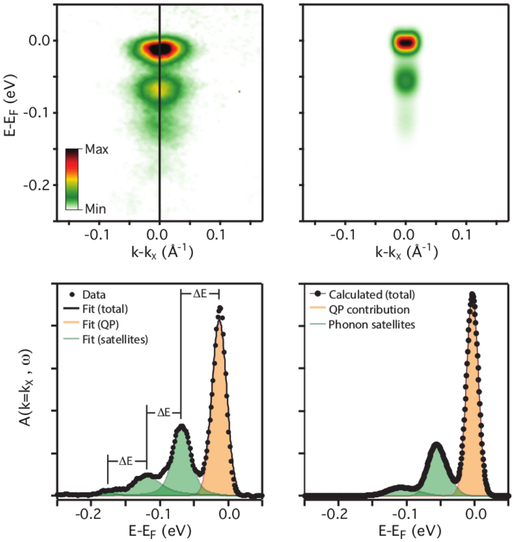
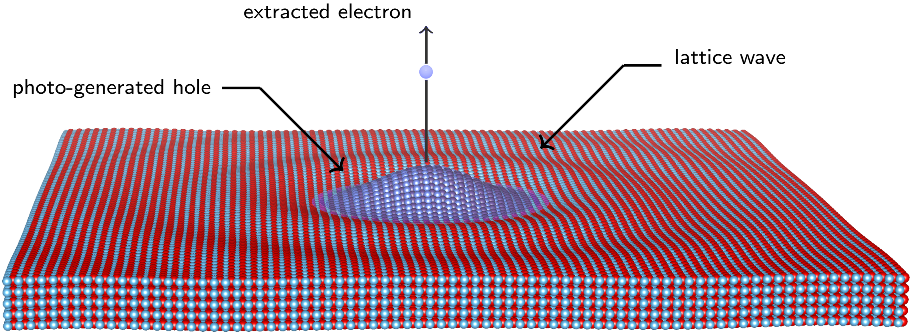


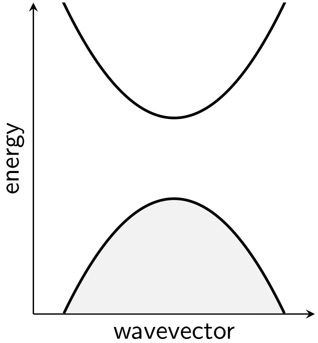
Figure from Riley et al,
Nat. Commun. 9, 2305 (2018)

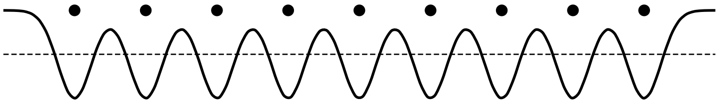
Meaning of satellite bands



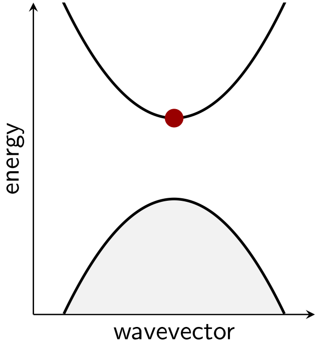
Phonon satellites are shake-up excitations

Electrons in solids: Bloch picture vs. Landau picture

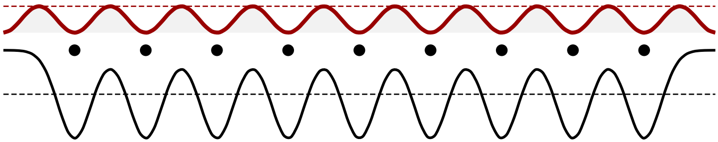




Electrons in solids: Bloch picture vs. Landau picture



band electron **delocalized**



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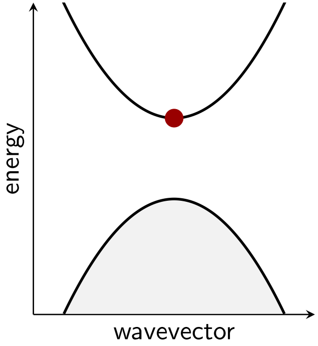
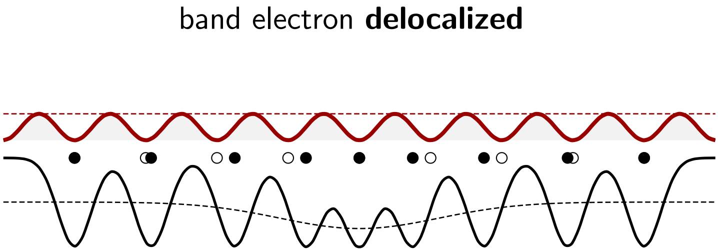
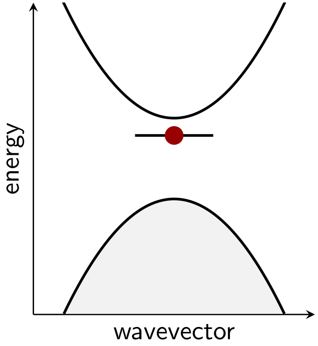
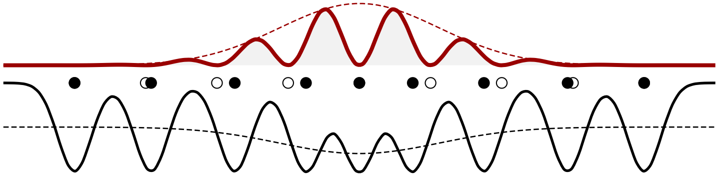






electron **localized** by lattice distortion: polaron



Electron aded to Li_2O_2 ground state

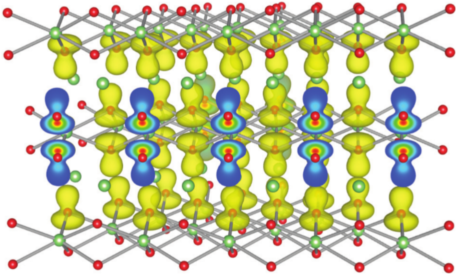


Figure from Feng et al, Phys. Rev. B 88, 184302 (2013)

Polarons in DFT calculations

Electron aded to Li_2O_2 ground state Self-localization after ionic relaxation

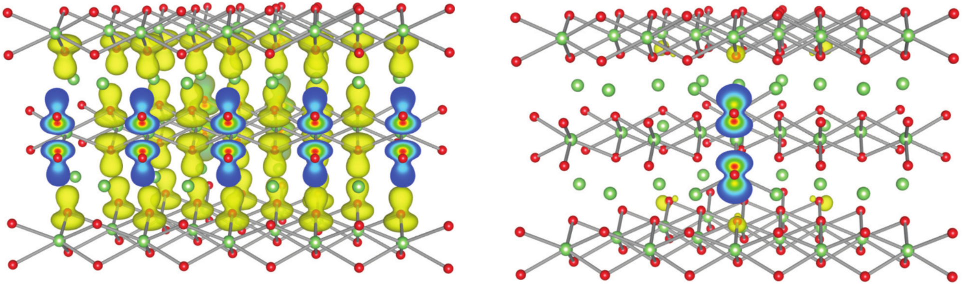


Figure from Feng et al, Phys. Rev. B 88, 184302 (2013)

Polarons in DFT calculations

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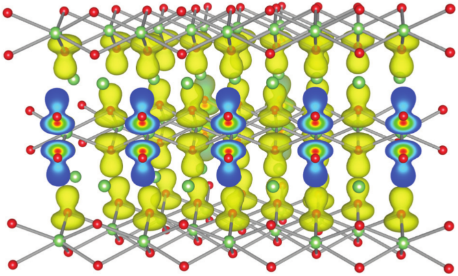
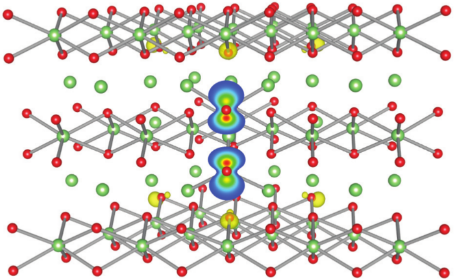


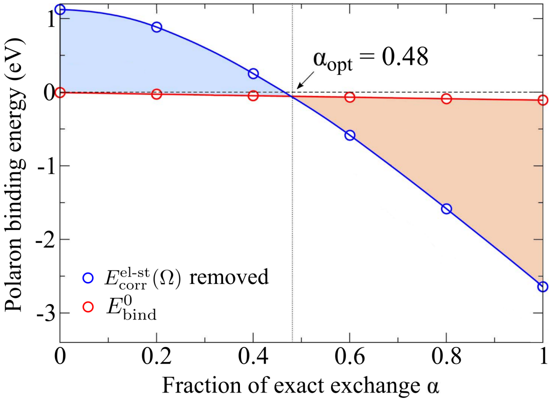
Self-localization after ionic relaxation

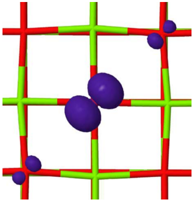


- Formation energy and size sensitive to the XC functional
- Only very small polarons accessible

Figure from Feng et al, Phys. Rev. B 88, 184302 (2013)

Sensitivity to functional: hole polaron in MgO

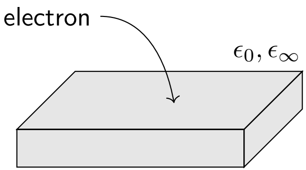




Figures adapted from Kokott, Levchenko, Rinke, Scheffler, New J. Phys. 20 (2018)

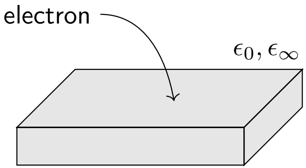
See Kokott et al for Koopman's based correction schemes

See Falletta et al, Phys. Rev. Lett. 129, 126401 (2022) for many-body self-interaction correction schemes



Pekar, Zh. Eksp. Teor. Fiz. 16, 341 (1946); Landau and Pekar, Zh. Eksp. Teor. Fiz. 18, 419 (1948)

Ground state of the polaron in the Landau-Pekar model



$$E = \frac{\hbar^2}{2m^*}\int d\mathbf{r}\,|\nabla\psi|^2 + \frac{1}{2}\int d\mathbf{r}\ \mathbf{E}\cdot\mathbf{D}$$

Pekar, Zh. Eksp. Teor. Fiz. 16, 341 (1946); Landau and Pekar, Zh. Eksp. Teor. Fiz. 18, 419 (1948)

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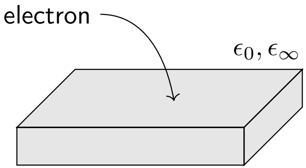

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$$\nabla\cdot\mathbf{D} = -e\big|\psi(\mathbf{r})\big|^2 \qquad \mathbf{D} = \varepsilon_0\epsilon_0\mathbf{E}$$

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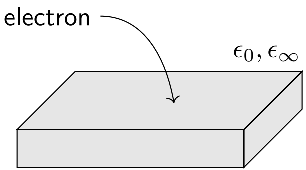

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$$\frac{1}{2}\int d\mathbf{r}\,\mathbf{E}\cdot\mathbf{D} = \frac{1}{2}\frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{\epsilon_0}\qquad\right)\int d\mathbf{r}\,d\mathbf{r}'\,\frac{|\psi(\mathbf{r})|^2|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}$$

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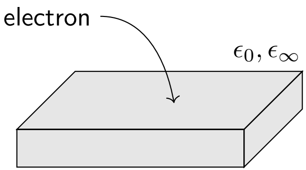

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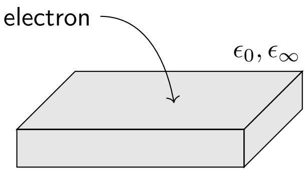

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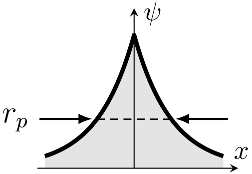
$$-\frac{\hbar^2}{2m^*}\nabla^2\psi(\mathbf{r}) - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon_\infty}\right)\int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}\psi(\mathbf{r}) = \varepsilon\,\psi(\mathbf{r})$$

Pekar, Zh. Eksp. Teor. Fiz. 16, 341 (1946); Landau and Pekar, Zh. Eksp. Teor. Fiz. 18, 419 (1948)

Simplest trial solution

$\psi(\mathbf{r}) = \exp(-|\mathbf{r}|/r_\mathrm{p})$



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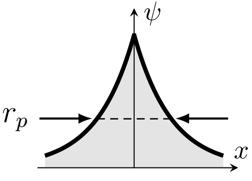
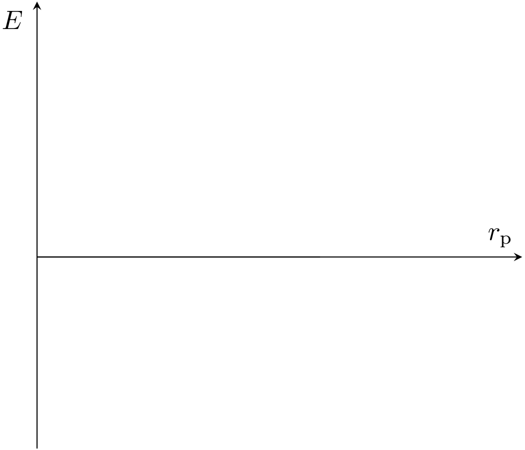


$E =$



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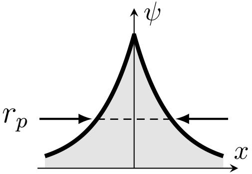
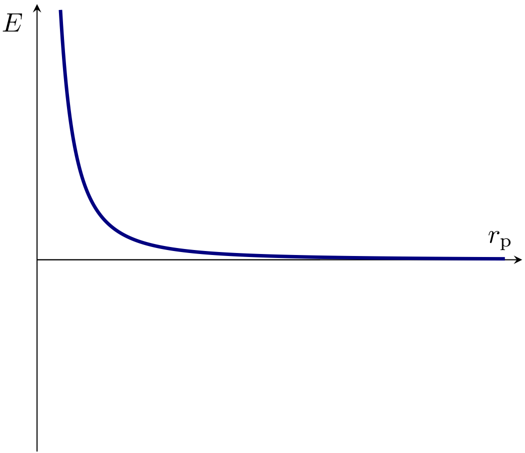


$$E = \frac{\hbar^2}{2m^*}\frac{1}{r_\mathrm{p}^2}$$



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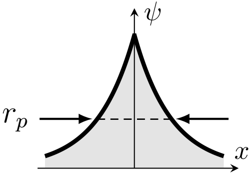
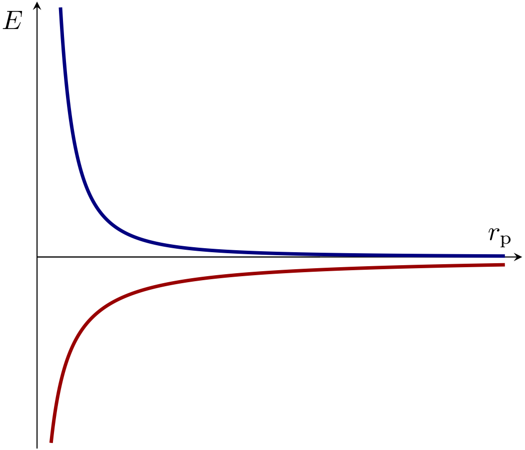


$$E = \frac{\hbar^2}{2m^*}\frac{1}{r_{\mathrm{p}}^2} - \frac{5}{16}\left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon_\infty}\right)\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_{\mathrm{p}}}$$



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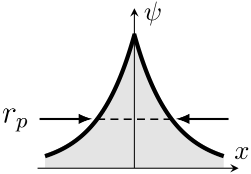

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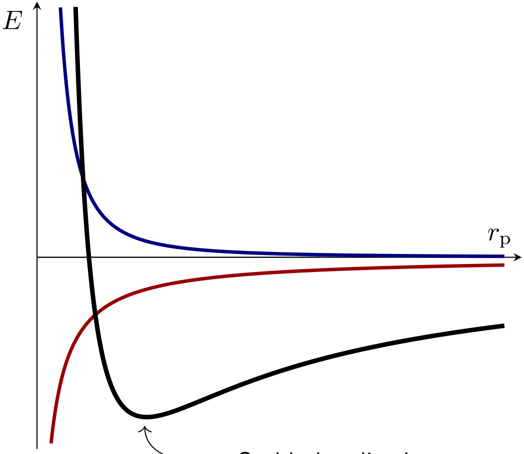
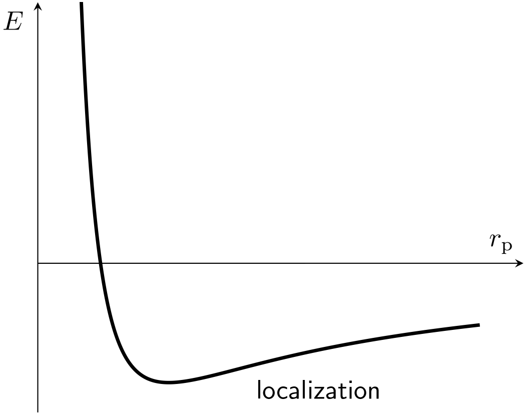


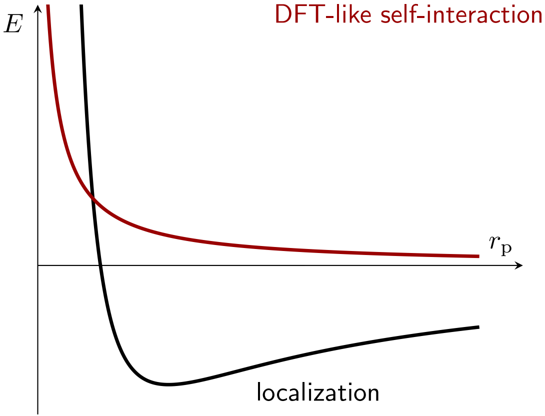
Effect of DFT self-interaction

$$-\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}$$



Effect of DFT self-interaction

$$-\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}\;+\;\int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}$$



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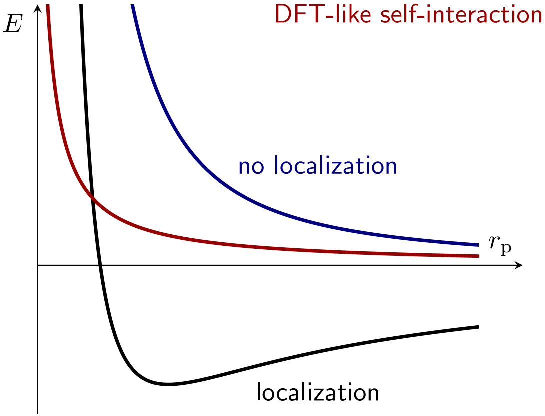
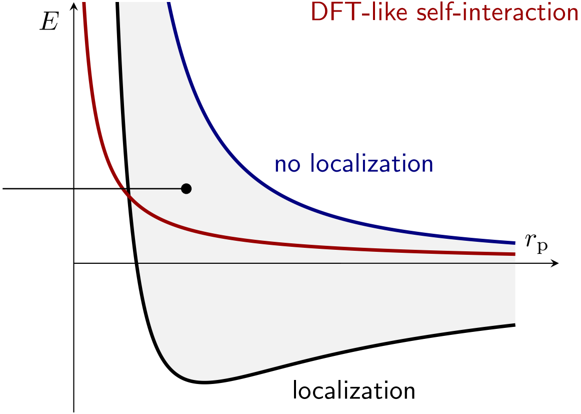


Effect of DFT self-interaction

$$-\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} + \int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}$$

Range spanned by varying α in hybrid functionals



Total energy in DFT

$$
\begin{aligned}
E &= \sum_{i\in\mathrm{occ}} \int d\mathbf{r} |\nabla\psi_i|^2 + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' \, \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + E_{xc}[n] \\
&+ \sum_{\kappa} \int d\mathbf{r} \, \frac{Z_\kappa n(\mathbf{r})}{|\mathbf{r}-\boldsymbol{\tau}_\kappa|} + \frac{1}{2}\sum_{\kappa\kappa'} \frac{Z_\kappa Z_{\kappa'}}{|\boldsymbol{\tau}_\kappa - \boldsymbol{\tau}_{\kappa'}|}
\end{aligned}
$$

Total energy in DFT

$$E = \sum_{i\in\text{occ}} \int d\mathbf{r} |\nabla\psi_i|^2 + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + E_{xc}[n]$$

$$+ \sum_{\kappa} \int d\mathbf{r} \frac{Z_\kappa n(\mathbf{r})}{|\mathbf{r}-\boldsymbol{\tau}_\kappa|} + \frac{1}{2}\sum_{\kappa\kappa'} \frac{Z_\kappa Z_{\kappa'}}{|\boldsymbol{\tau}_\kappa - \boldsymbol{\tau}_{\kappa'}|}$$

Add one electron

$$n(\mathbf{r}) \to n(\mathbf{r}) + |\psi(\mathbf{r})|^2$$

$$\boldsymbol{\tau}_\kappa \to \boldsymbol{\tau}_\kappa + \mathbf{u}_\kappa$$

Total energy in DFT

$$E =$$

$$E = \sum_{i\in \mathrm{occ}} \int d\mathbf{r} |\nabla \psi_i|^2 + \int d\mathbf{r} |\nabla \psi|^2$$

Total energy in DFT

$$
\begin{aligned}
E &= \sum_{i\in\text{occ}} \int d\mathbf{r} |\nabla \psi_i|^2 + \int d\mathbf{r} |\nabla \psi|^2 \\
&+ \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \frac{[n(\mathbf{r}) + |\psi(\mathbf{r})|^2]\,[n(\mathbf{r}') + |\psi(\mathbf{r}')|^2]}{|\mathbf{r}-\mathbf{r}'|} + E_{xc}[n + |\psi|^2]
\end{aligned}
$$

$$
\begin{aligned}
E &= \sum_{i\in\text{occ}} \int d\mathbf{r} |\nabla \psi_i|^2 + \int d\mathbf{r} |\nabla \psi|^2 \\
&+ \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \frac{\left[n(\mathbf{r}) + |\psi(\mathbf{r})|^2\right]\left[n(\mathbf{r}') + |\psi(\mathbf{r}')|^2\right]}{|\mathbf{r}-\mathbf{r}'|} + E_{xc}[n + |\psi|^2] \\
&+ \sum_{\kappa} \int d\mathbf{r} \frac{Z_\kappa \left[n(\mathbf{r}) + |\psi(\mathbf{r})|^2\right]}{|\mathbf{r} - (\boldsymbol{\tau}_\kappa + \mathbf{u}_\kappa)\,|} + \frac{1}{2}\sum_{\kappa\kappa'} \frac{Z_\kappa Z_{\kappa'}}{|\,(\boldsymbol{\tau}_\kappa + \mathbf{u}_\kappa) - (\boldsymbol{\tau}_{\kappa'} + \mathbf{u}_{\kappa'})\,|}
\end{aligned}
$$

Polarons in density-functional perturbation theory

Formation energy functional of an extra electron, without self-interaction

$$E = \int d\mathbf{r}\, \psi^* \hat{H}_{\mathrm{KS}}\, \psi \;+ \int d\mathbf{r}\, |\psi|^2 \, \frac{\partial V_{\mathrm{KS}}}{\partial \boldsymbol{\tau}_\kappa} \cdot \mathbf{u}_\kappa + \frac{1}{2} \mathbf{u}_\kappa \cdot \mathbf{C}_{\kappa\kappa'} \cdot \mathbf{u}_{\kappa'}$$

Formation energy functional of an extra electron, without self-interaction

$$E = \int d\mathbf{r}\, \psi^* \hat{H}_{\rm KS}\, \psi \; + \int d\mathbf{r}\, |\psi|^2 \frac{\partial V_{\rm KS}}{\partial \boldsymbol{\tau}_\kappa} \cdot \mathbf{u}_\kappa + \frac{1}{2} \mathbf{u}_\kappa \cdot \mathbf{C}_{\kappa\kappa'} \cdot \mathbf{u}_{\kappa'}$$

Variational minimization with respect to ψ and $\mathbf{u}_\kappa$

$$\begin{cases} \hat{H}_{\rm KS}\, \psi + \; \psi\, \dfrac{\partial V_{\rm KS}}{\partial \boldsymbol{\tau}_\kappa} \cdot \mathbf{u}_\kappa = \lambda\, \psi \\ \mathbf{u}_\kappa = -(\mathbf{C})^{-1}_{\kappa\kappa'} \cdot \displaystyle\int d\mathbf{r}\, \frac{\partial V_{\rm KS}}{\partial \boldsymbol{\tau}_{\kappa'}}\, |\psi|^2 \end{cases}$$

Polarons in reciprocal space

$$\psi(\mathbf{r}) = \frac{1}{N_p} \sum_{n\mathbf{k}} A_{n\mathbf{k}} \, \psi_{n\mathbf{k}}(\mathbf{r})$$

$$\mathbf{u}_\kappa(\mathbf{R}) = -\frac{2}{N_p} \sum_{\mathbf{q}\nu} B^*_{\mathbf{q}\nu} \sqrt{\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}\nu}}} \, e^{i\mathbf{q}\cdot\mathbf{R}} \, \mathbf{e}_{\kappa,\mathbf{q}\nu}$$

Theory in Sio et al, Phys. Rev. Lett. 122, 246403 (2019)

Polarons in reciprocal space

$$\psi(\mathbf{r}) = \frac{1}{N_p} \sum_{n\mathbf{k}} A_{n\mathbf{k}} \, \psi_{n\mathbf{k}}(\mathbf{r})$$

$$\mathbf{u}_\kappa(\mathbf{R}) = -\frac{2}{N_p} \sum_{\mathbf{q}\nu} B^*_{\mathbf{q}\nu} \sqrt{\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}\nu}}} \, e^{i\mathbf{q}\cdot\mathbf{R}} \, \mathbf{e}_{\kappa,\mathbf{q}\nu}$$

$$\frac{2}{N_p} \sum_{\mathbf{q}m\nu} B_{\mathbf{q}\nu} \, g^*_{mn\nu}(\mathbf{k},\mathbf{q}) \, A_{m\mathbf{k}+\mathbf{q}} = (\varepsilon_{n\mathbf{k}} - \varepsilon) \, A_{n\mathbf{k}}$$

$$B_{\mathbf{q}\nu} = \frac{1}{N_p} \sum_{mn\mathbf{k}} A^*_{m\mathbf{k}+\mathbf{q}} \, \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\omega_{\mathbf{q}\nu}} \, A_{n\mathbf{k}}$$

Ab initio polaron equations

Theory in Sio et al, Phys. Rev. Lett. 122, 246403 (2019)

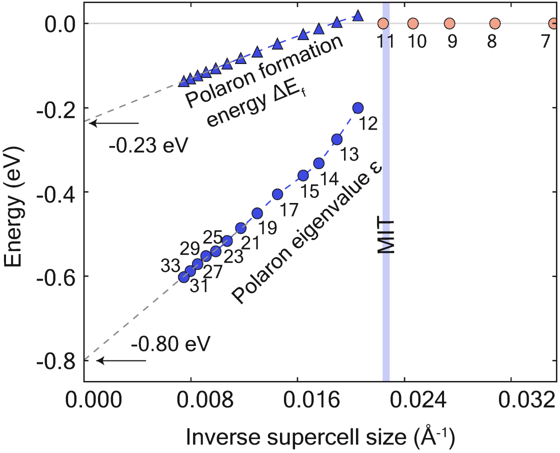
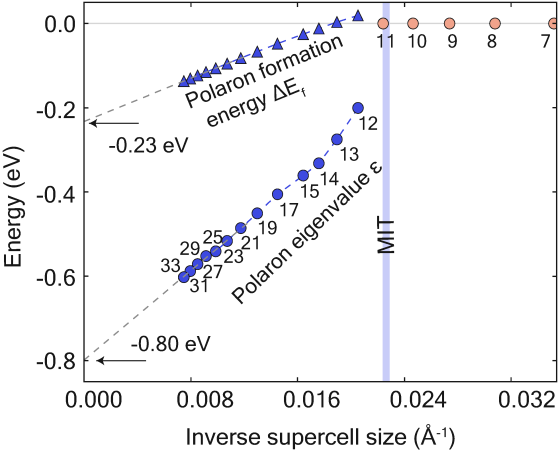


Figure from Sio et al, PRL 122, 246403 (2019)



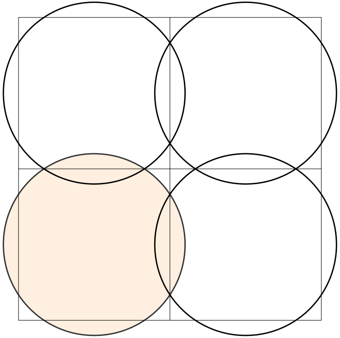


Figure from Sio et al, PRL 122, 246403 (2019)

Electron polaron in LiF

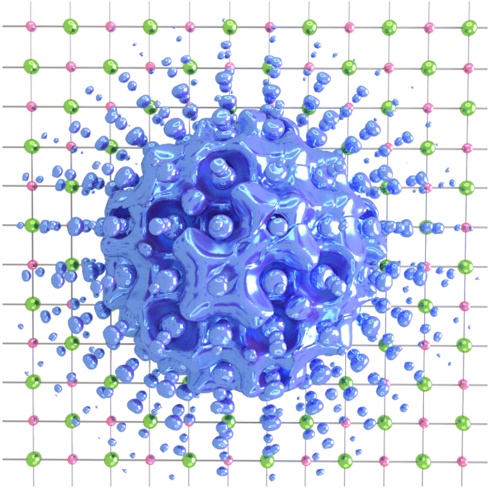
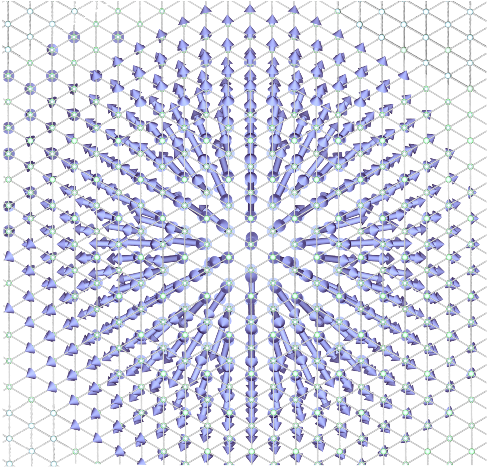


Figure from Sio et al, PRL 122, 246403 (2019)

Electron polaron in LiF



fluorine displacements

Figure from Sio et al, PRL 122, 246403 (2019)

Hole polaron in LiF

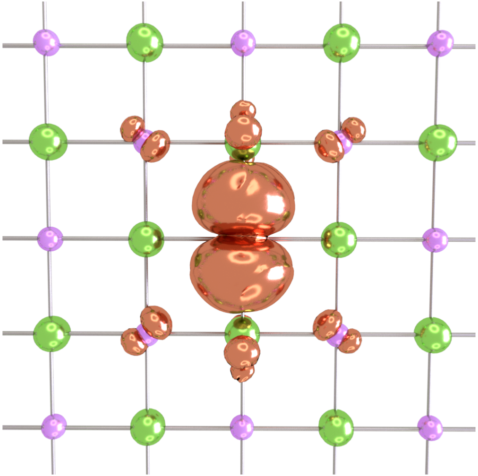
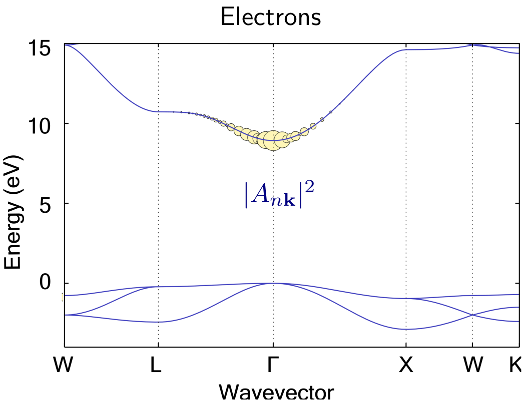
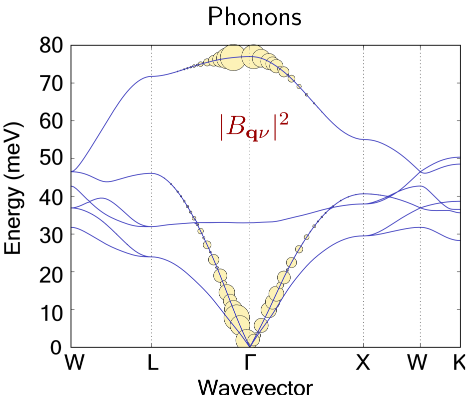


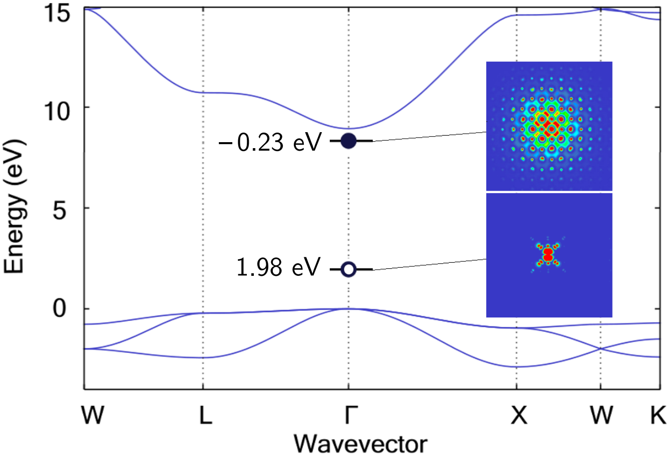
Figure from Sio et al, PRB 99, 235139 (2019)

Electron polaron in LiF



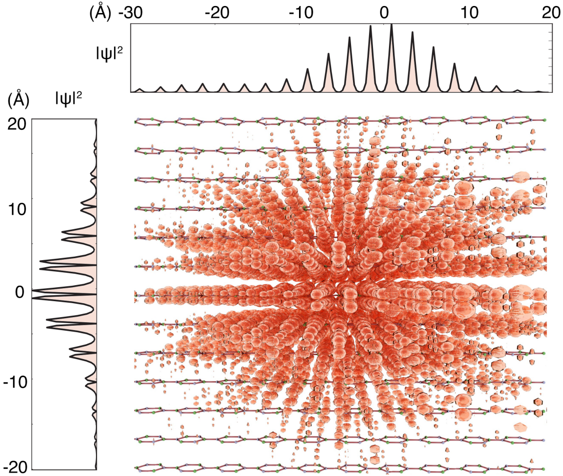


Quasiparticle energies of polarons in LiF



Shown are formation energies w.r.t. delocalized solutions

Hole polaron in bulk h-BN



Formation energy

–13.6 meV

Figure from Sio et al, Nat. Phys. 19, 629 (2023)

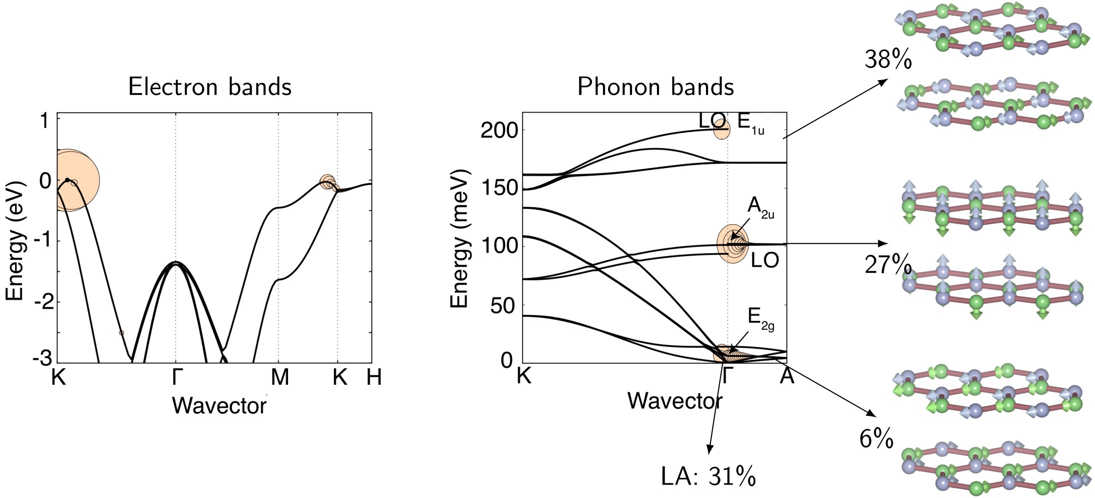
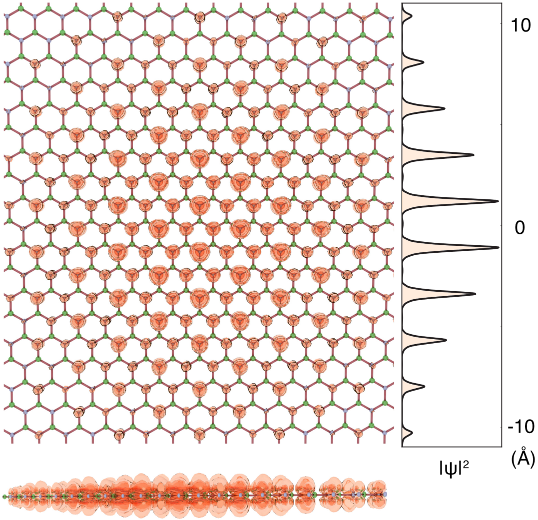


Figure from Sio et al, Nat. Phys. 19, 629 (2023)

Formation energy
–15.9 meV



Hole polaron in monolayer h-BN

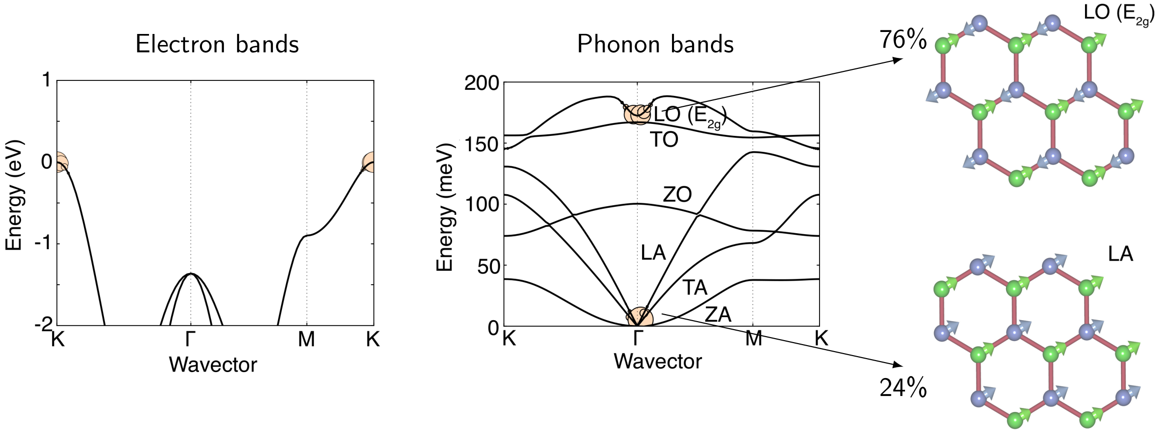


Figure from Sio et al, Nat. Phys. 19, 629 (2023)

Many-body field-theoretic approach to polarons

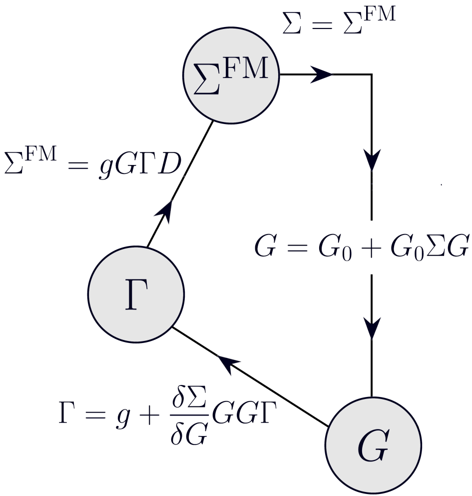


Figure from Lafuente-Bartolomé et al, Phys. Rev. Lett. 129, 076402 (2022)

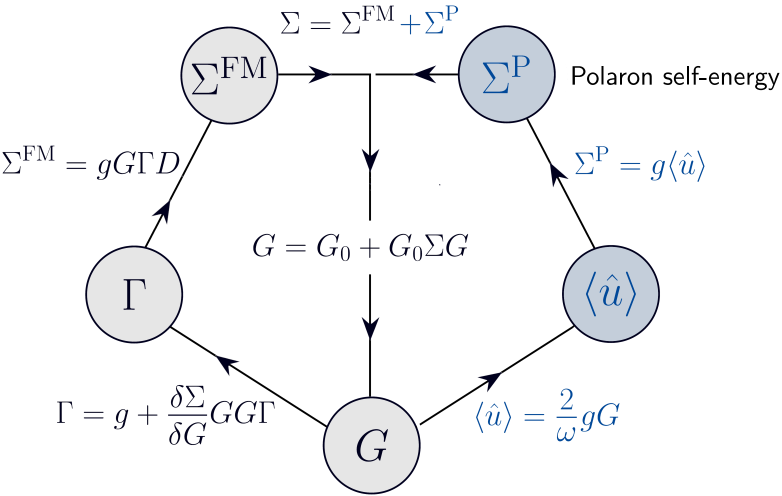


Figure from Lafuente-Bartolomé et al, Phys. Rev. Lett. 129, 076402 (2022)

Lehmann representation of the Green's function

$$G(\mathbf{r},\mathbf{r}';\omega) = \sum_s \frac{f_s(\mathbf{r}) f_s^*(\mathbf{r}')}{\hbar\omega - \varepsilon_s}$$

⟶

Dyson orbitals

$$f_s(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{n\mathbf{k}} A^s_{n\mathbf{k}}\, \psi_{n\mathbf{k}}(\mathbf{r})$$

From Lafuente-Bartolomé at al, PRB 106, 075119 (2022)

Many-body field-theoretic approach to polarons

Lehmann representation of the Green's function

$$G(\mathbf{r},\mathbf{r}';\omega) = \sum_s \frac{f_s(\mathbf{r}) f_s^*(\mathbf{r}')}{\hbar\omega - \varepsilon_s}$$

$\longrightarrow$

Dyson orbitals

$$f_s(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{n\mathbf{k}} A^s_{n\mathbf{k}}\, \psi_{n\mathbf{k}}(\mathbf{r})$$

$$\sum_{n'\mathbf{k}'} \left[\varepsilon_{n\mathbf{k}}\, \delta_{n\mathbf{k},n'\mathbf{k}'} + \Sigma^{\mathrm{FM}}_{n\mathbf{k},n'\mathbf{k}'}(\varepsilon_s) + \Sigma^{\mathrm{P}}_{n\mathbf{k},n'\mathbf{k}'} \right] A^s_{n'\mathbf{k}'} = \varepsilon_s\, A^s_{n\mathbf{k}}$$

Many-body *ab initio* polaron equations

From Lafuente-Bartolomé at al, PRB 106, 075119 (2022)

Comparison with Diagrammatic Monte Carlo

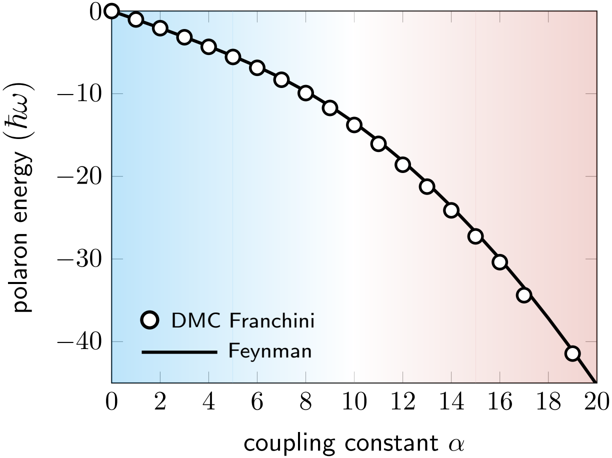


Figure from Lafuente-Bartolomé et al, Phys. Rev. Lett. 129, 076402 (2022)

Diagrammatic Monte Carlo data from: Hahn, Klimin, Tempere, Devreese, Franchini, Phys. Rev. B 97, 134305 (2018)

Comparison with Diagrammatic Monte Carlo

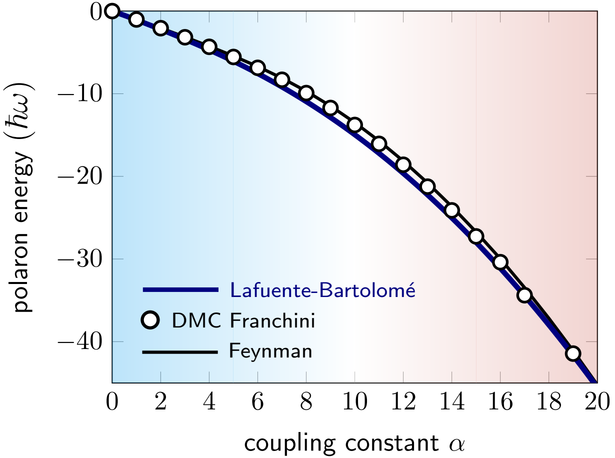
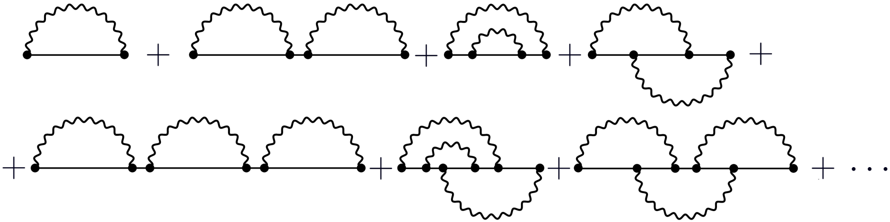


Figure from Lafuente-Bartolomé et al, Phys. Rev. Lett. 129, 076402 (2022)

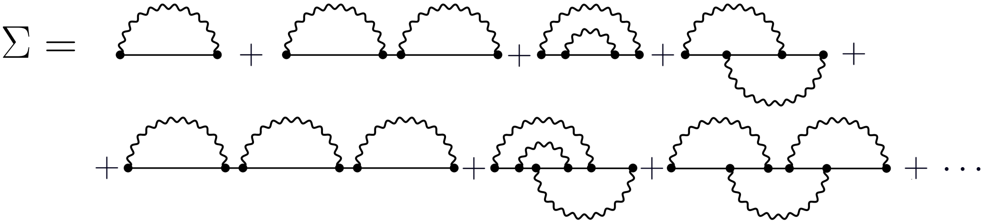
Diagrammatic Monte Carlo data from: Hahn, Klimin, Tempere, Devreese, Franchini, Phys. Rev. B 97, 134305 (2018)

Diagrammatic Monte Carlo

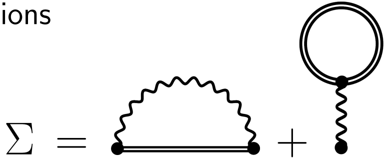
$\Sigma =$



Diagrammatic Monte Carlo



Many-body polaron equations



Take-home messages

- DFT calculations of polarons suffer from the self-interaction error
- *Ab initio* polaron equations yield self-interaction-free polaron energies and wavefunctions
- These equations are the DFT approximation to a many-body Green's formalism related to the theory discussed on Monday
- There are many types of polarons, from atomic-like polarons to very large nanoscale polarons

References

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- Devreese and Alexandrov, Rep. Prog. Phys. 72, 066501 (2009) [link]
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- Falletta and Pasquarello, Phys. Rev. B 106, 125119 (2022) [link]