2021 Virtual School on Electron-Phonon Physics and the EPW code

June 14-18 2021

Lecture Thu.2

Polarons from first principles

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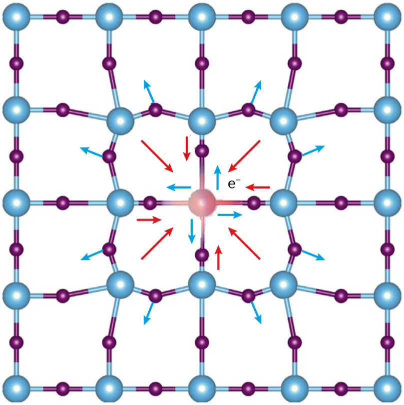
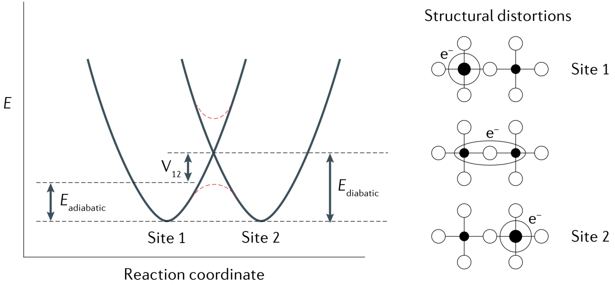
The University of Texas at Austin

Lecture Summary

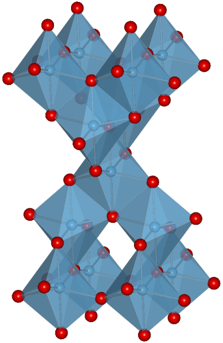
- Introduction to the polaron concept
- Photoemission signatures of polarons
- Many-body calculations of polaron satellites
- DFT calculations of polarons
- *Ab initio* polaron equations
- Open questions in polaron physics

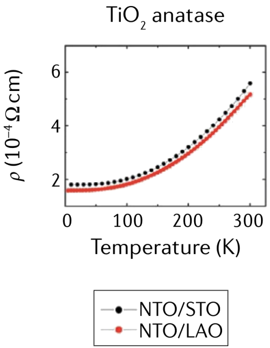
Intuitive notion of polaron

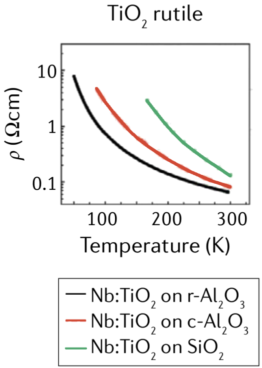


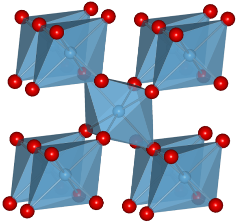


Figures from Franchini et al, Nat. Rev. Mater. 2021, 10.1038/s41578-021-00289-w









Diffusive

Activated

Hall mobility data from Zhang et al, J. Appl. Phys. 102, 013701 (2007);
see discussion in Franchini et al, Nat. Rev. Mater. 2021, 10.1038/s41578-021-00289-w

Angle-resolved photoelectron spectroscopy (ARPES)

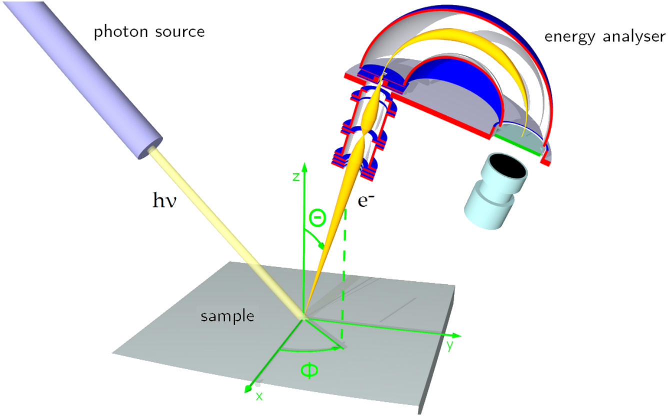
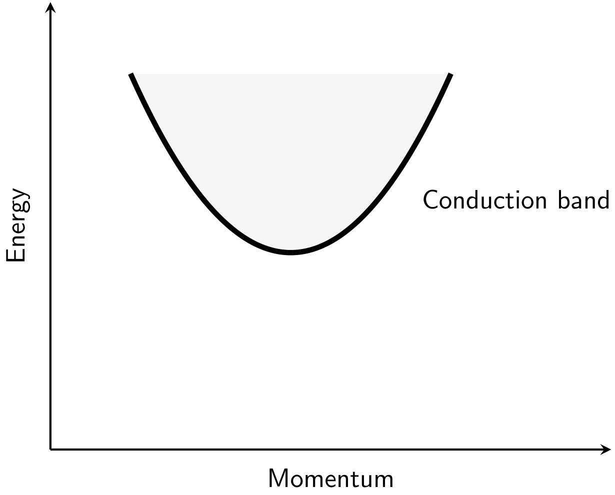
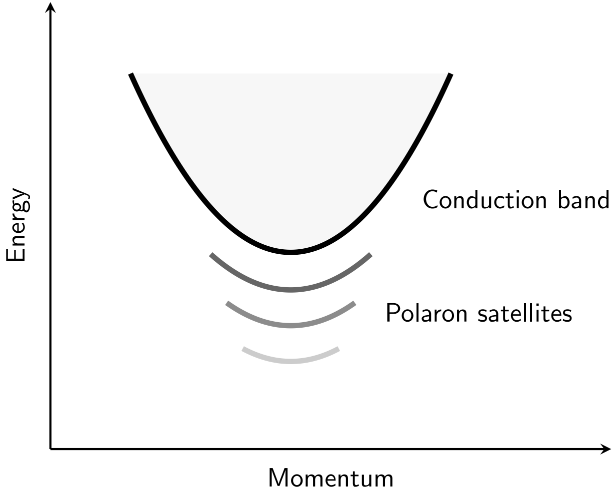


Figure from commons.wikimedia.org/wiki/File:ARPESgeneral.png

Polaron satellites



Polaron satellites



Polaron satellites in anatase TiO_2

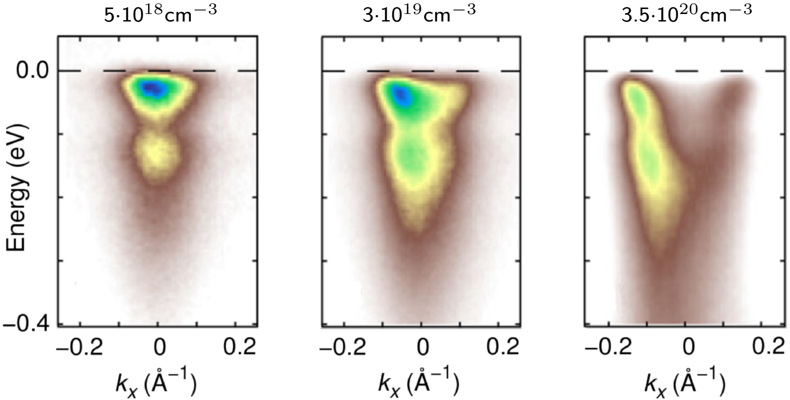


Figure from Moser et al, Phys. Rev. Lett. 110, 196403 (2013)

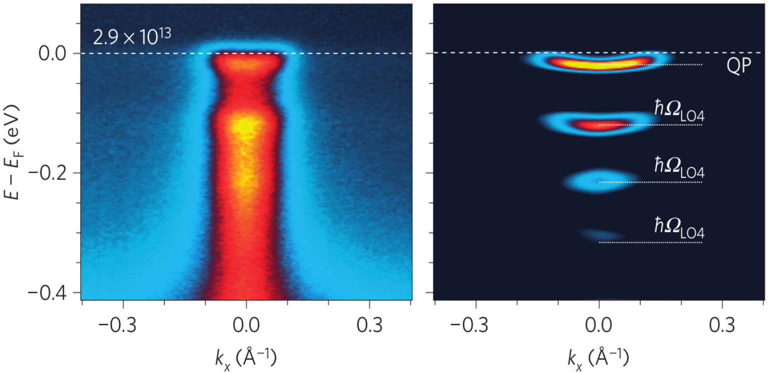


Figure from Wang et al, Nature Mater. 15, 835 (2016)

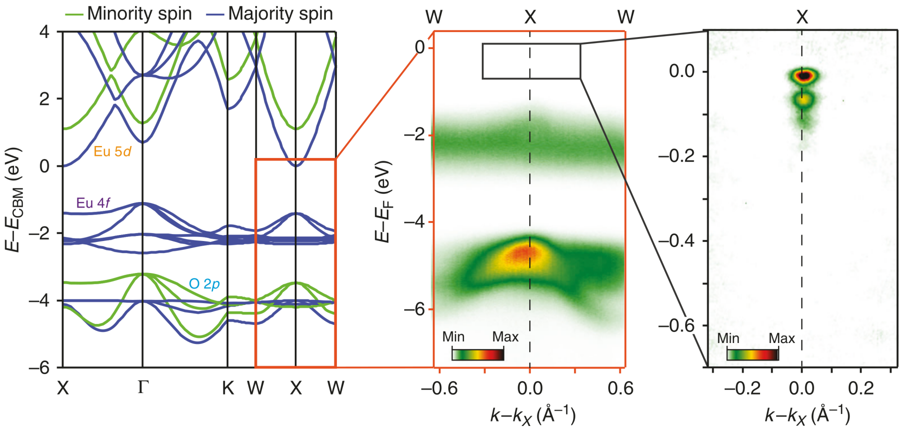


Figure from Riley et al, Nat. Commun. 9, 2305 (2018)

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

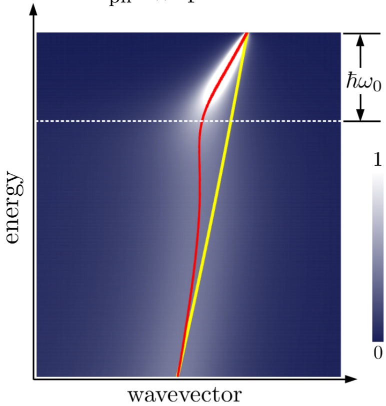


Figure from FG, Rev. Mod. Phys. 89, 015003 (2017)

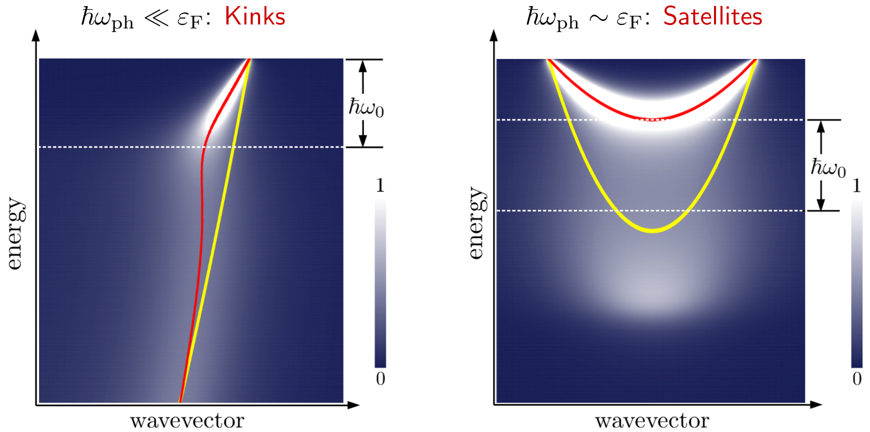


Figure from FG, Rev. Mod. Phys. 89, 015003 (2017)

Many-body viewpoint

Quasiparticle equation (from Lecture Tue.2)

$$\left[-\frac{\hbar^2}{2m_\mathrm{e}}\nabla^2 + V_\mathrm{tot}(\mathbf{r})\right] f_s(\mathbf{x}) + \int d\mathbf{x}' \, \underline{\Sigma(\mathbf{x},\mathbf{x}',\varepsilon_s/\hbar)} \, f_s(\mathbf{x}') = \varepsilon_s f_s(\mathbf{x})$$

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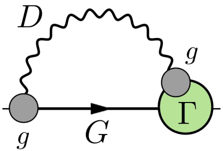
$\Sigma =$ 

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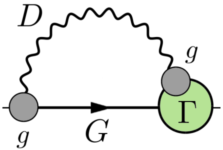
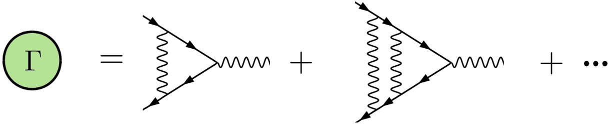
$\Sigma =$ 

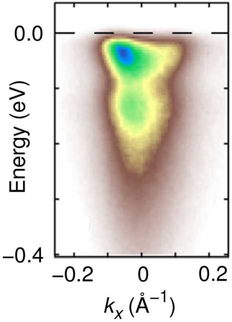


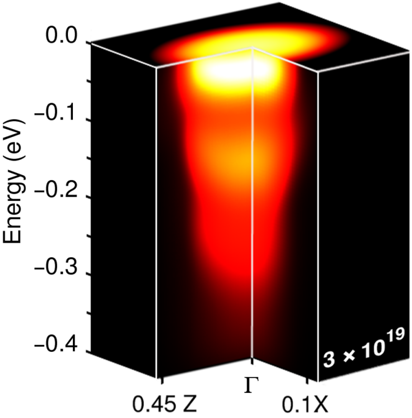
Cumulant expansion method

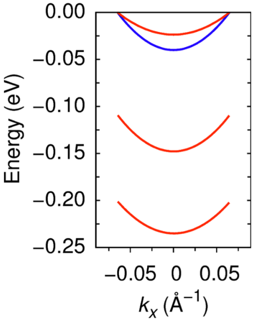
Aryasetiawan et al, Phys. Rev. Lett. 77, 2268 (1996); Zhou et al, J. Chem. Phys. 143, 184109 (2015); Gumhalter et al, Phys. Rev. B 94, 035103 (2016); Nery et al, Phys. Rev. B 97 (2018)

Calculated vs. measured spectral function: TiO_2

Moser et al,
PRL 110, 196403 (2013)



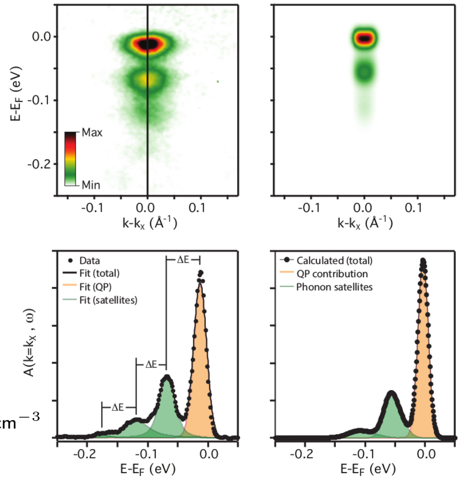




Verdi et al, Nat. Commun. 8, 15769 (2017)

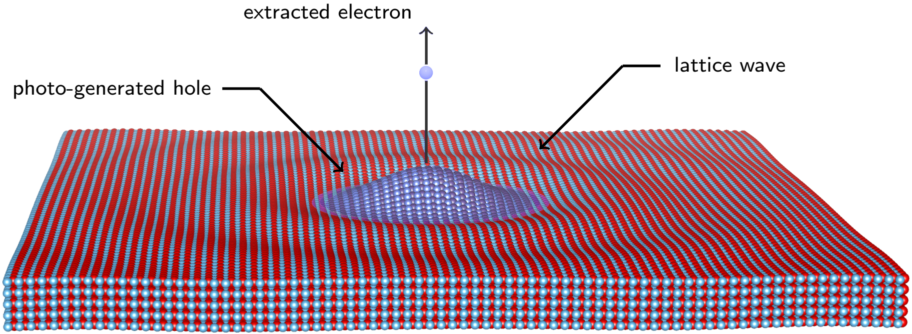
Calculated vs. measured spectral function: EuO

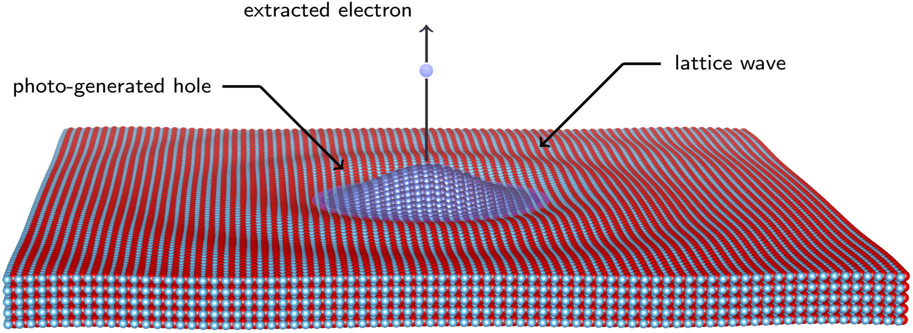
$n = 10^{17}$ cm^{-3}



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

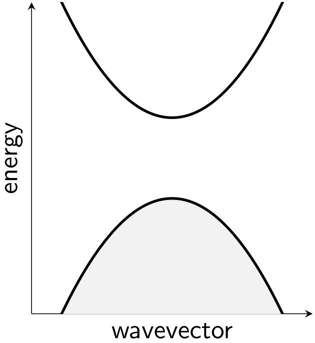
Meaning of satellite bands

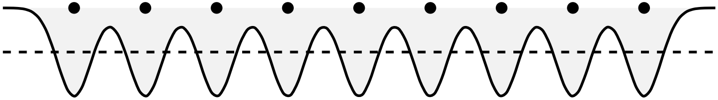




Satellites are shake-up excitations, the polaron is the QP peak

Electron localization





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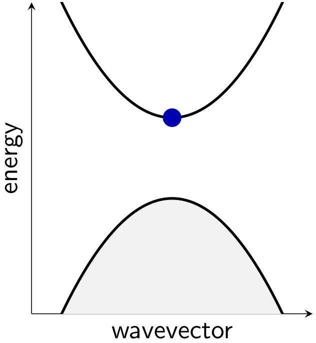
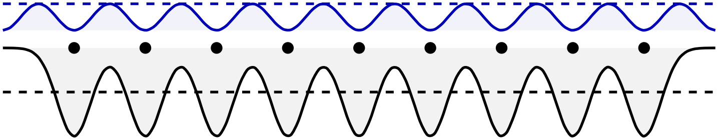
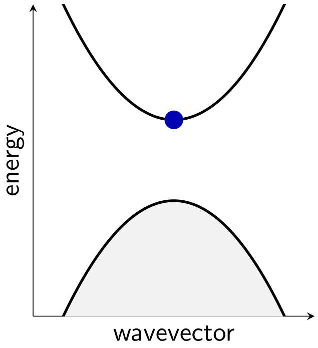
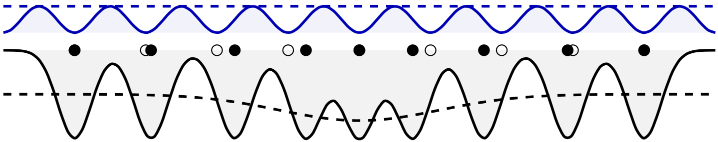





energy
wavevector



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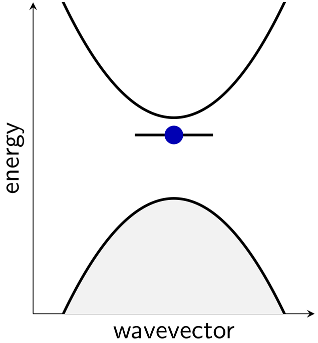

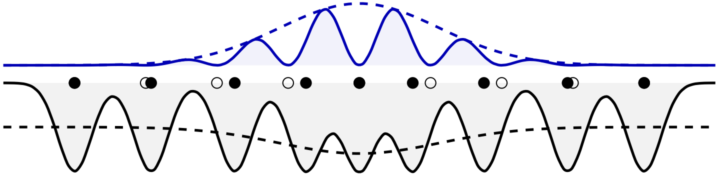

Ground state of the polaron in the Landau-Pekar model

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

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

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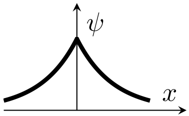
$$-\frac{\hbar^2}{2m^*}\nabla^2\psi(\mathbf{r}) - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon_\infty}\right)\int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}\psi(\mathbf{r}) = \varepsilon\,\psi(\mathbf{r})$$

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

Simplest trial solution: $\psi(\mathbf{r}) = \exp(-|\mathbf{r}|/r_{\rm p})$



Landau-Pekar equation

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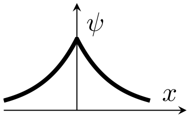
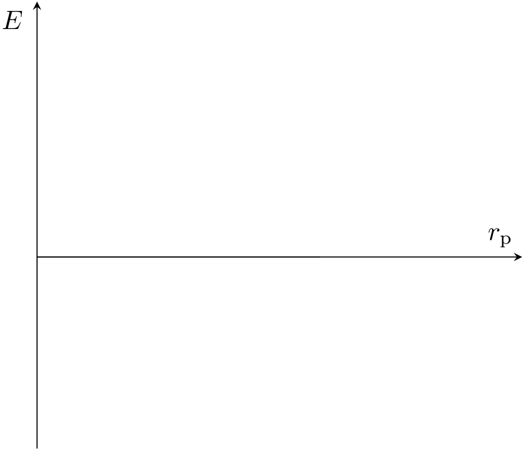


$E =$



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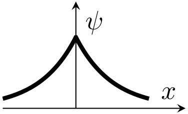
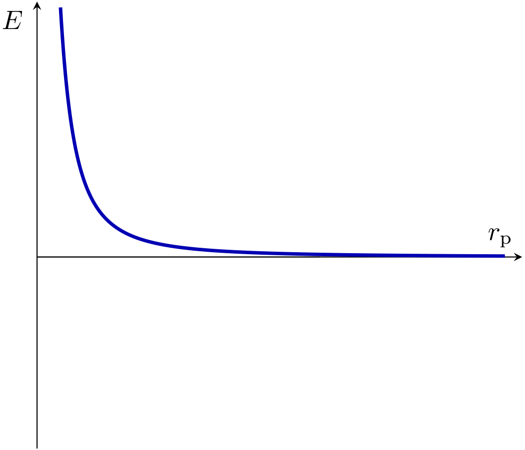


$$E = \frac{\hbar^2}{2m^*}\frac{1}{r_{\mathrm{p}}^2}$$



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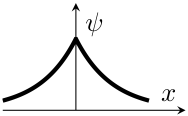
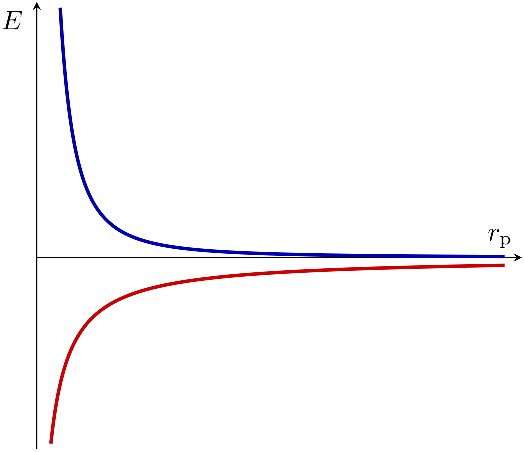


$$E = \frac{\hbar^2}{2m^*}\frac{1}{r_\mathrm{p}^2} - \frac{5}{16}\left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon_\infty}\right)\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_\mathrm{p}}$$



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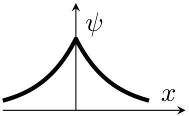

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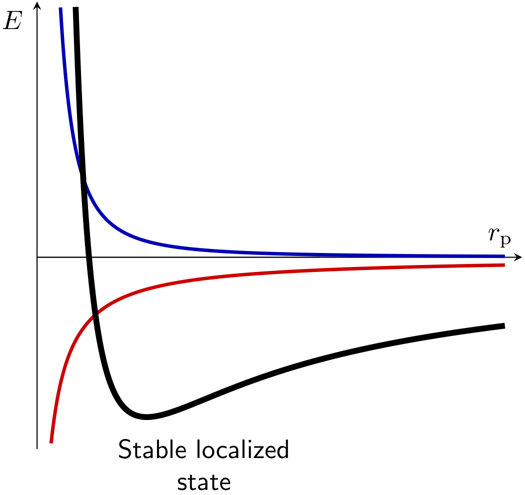
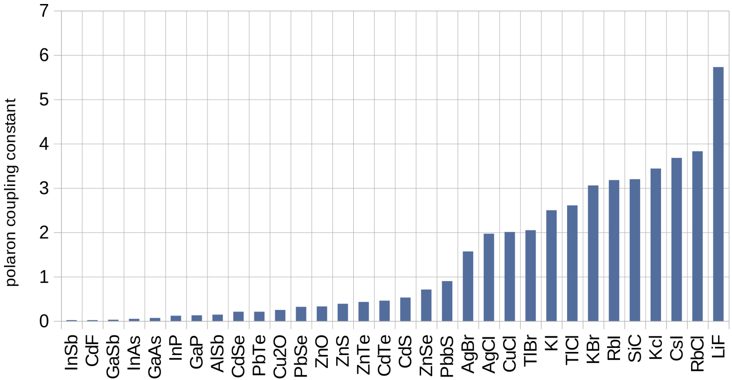


The polaron coupling constant

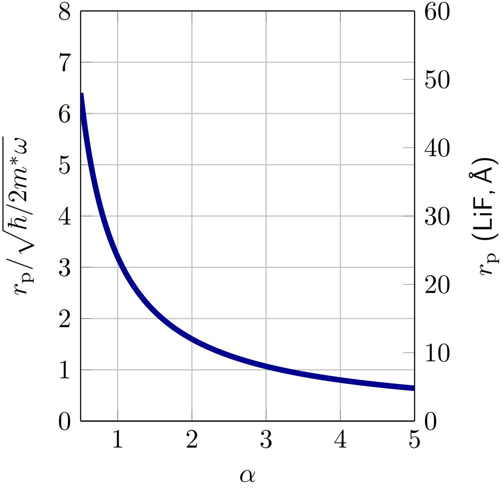
$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar}\sqrt{\frac{m^*}{2\hbar\omega}}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)$$



Data from Iadonisi, Riv. Nuovo Cim. 7, 1 (1984)

Size of a polaron in the Landau-Pekar model

Radius: $r_{\mathrm{p}} = \frac{16}{5}\sqrt{\frac{\hbar}{2m^*\omega}}\,\frac{1}{\alpha}$



Electron aded to Li_2O_2 ground state

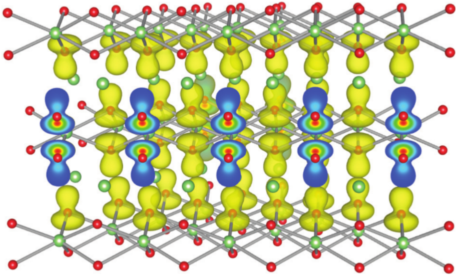


Figure from Feng et al, Phys. Rev. B 88, 184302 (2013)

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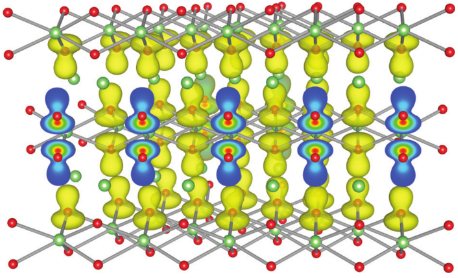


Self-localization after ionic relaxation

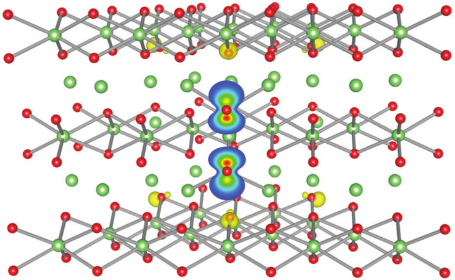
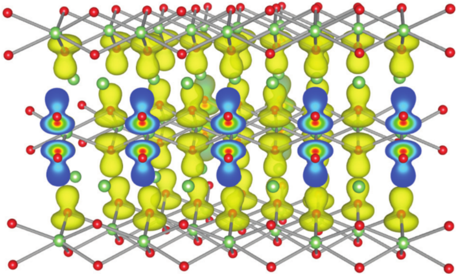


Figure from Feng et al, Phys. Rev. B 88, 184302 (2013)

Polarons in DFT calculations

Electron aded to Li_2O_2 ground state



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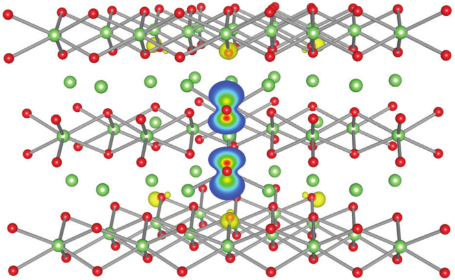

Challenges { The energy and size of the localized state are sensitive to the XC functional
Only small polarons accessible

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

Total energy in DFT

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

Total energy in DFT

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\end{aligned}
$$

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

$$E =$$

Total energy in DFT

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

Total energy in DFT

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

Total energy in DFT

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

Denny Sio

Total Energy functional of an extra electron or hole, without self-interaction

$$E = \int d\mathbf{r}\, \psi^* \hat{H}_{\mathrm{KS}}\, \psi + \int d\mathbf{r}\, \frac{\partial V_{\mathrm{KS}}}{\partial \tau_{\kappa\alpha}}\, |\psi|^2\, u_{\kappa\alpha} + \frac{1}{2} C_{\kappa\alpha,\kappa'\alpha'} u_{\kappa\alpha} u_{\kappa'\alpha'}$$

Denny Sio

Total Energy functional of an extra electron or hole, without self-interaction

$$E = \int d\mathbf{r}\, \psi^* \hat{H}_{\rm KS}\, \psi + \int d\mathbf{r}\, \frac{\partial V_{\rm KS}}{\partial \tau_{\kappa\alpha}} |\psi|^2\, u_{\kappa\alpha} + \frac{1}{2} C_{\kappa\alpha,\kappa'\alpha'} u_{\kappa\alpha} u_{\kappa'\alpha'}$$

Variational minimization with respect to ψ and $u_{\kappa\alpha}$

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

Polarons in reciprocal space

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

$$u_{\kappa\alpha}(\mathbf{R}) = -\frac{2}{N_p}\sum_{\mathbf{q}\nu} B^*_{\mathbf{q}\nu}\left(\frac{\hbar}{2M_\kappa\omega_{\mathbf{q}\nu}}\right)^{1/2} e_{\kappa\alpha,\mathbf{q}\nu}\; e^{i\mathbf{q}\cdot\mathbf{R}}$$

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

$$u_{\kappa\alpha}(\mathbf{R}) = -\frac{2}{N_p}\sum_{\mathbf{q}\nu} B^*_{\mathbf{q}\nu}\left(\frac{\hbar}{2M_\kappa\omega_{\mathbf{q}\nu}}\right)^{1/2} e_{\kappa\alpha,\mathbf{q}\nu}\; e^{i\mathbf{q}\cdot\mathbf{R}}$$

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

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

Ab initio polaron equations

Electron polaron in LiF

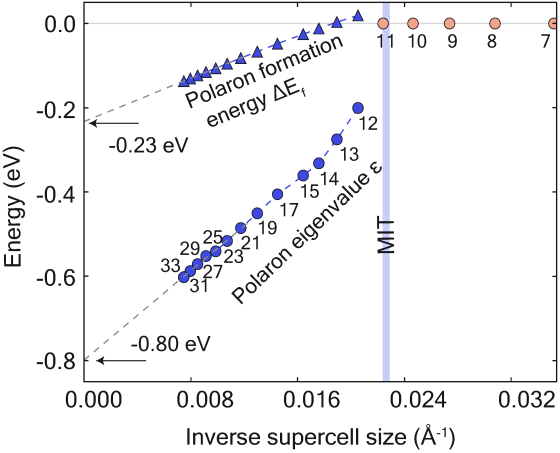
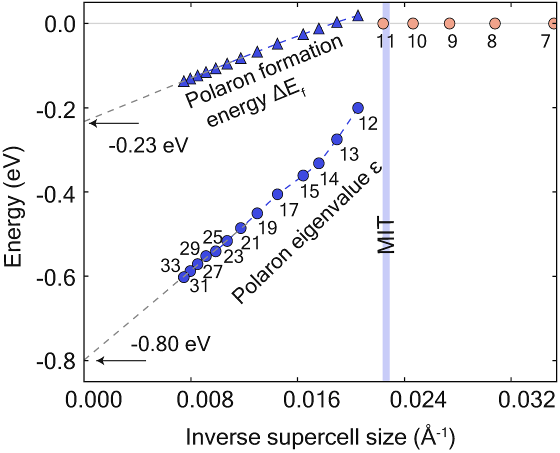


Figure from Sio et al, PRL 122, 246403 (2019)



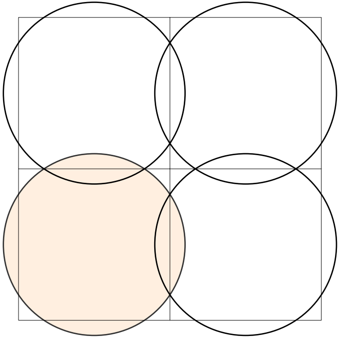


Figure from Sio et al, PRL 122, 246403 (2019)

Electron polaron in LiF

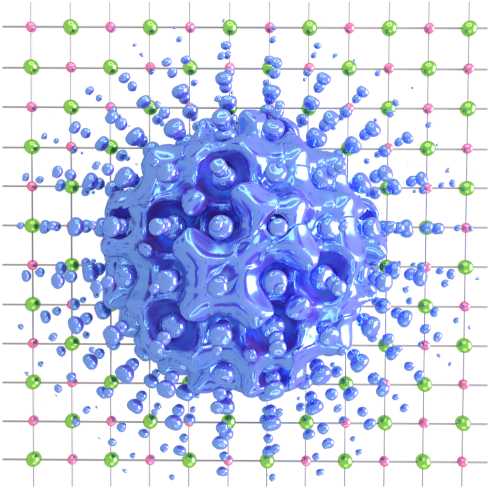
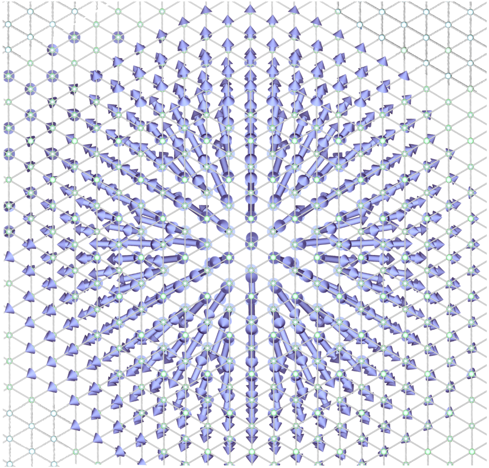


Figure from Sio et al, PRL 122, 246403 (2019)

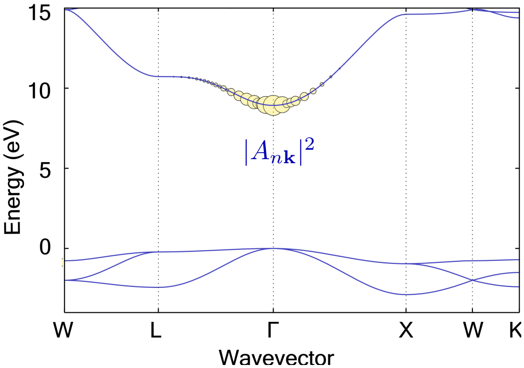


fluorine displacements

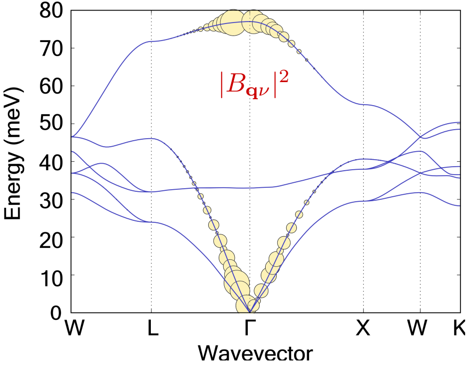
Figure from Sio et al, PRL 122, 246403 (2019)

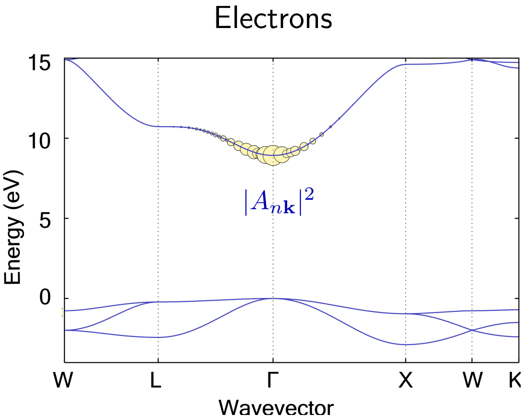
Example: Electron polaron in Lithium Fluoride

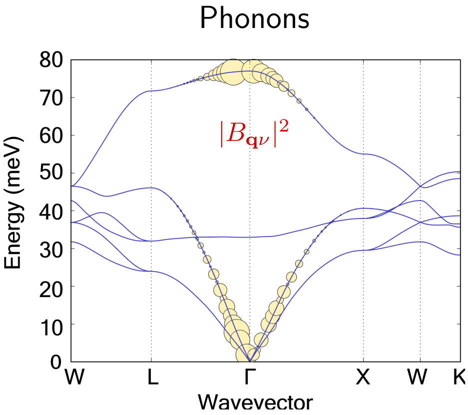
Electrons



Phonons







Fröhlich polaron

Hole polaron in LiF

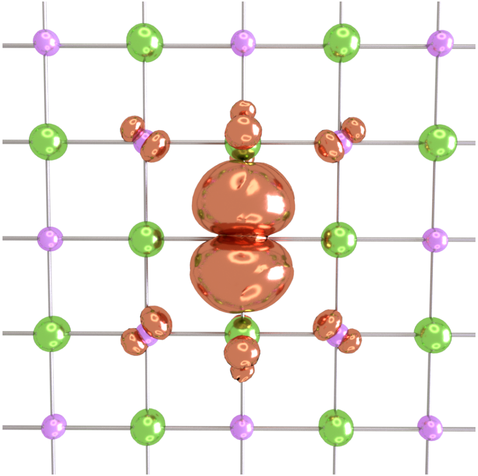
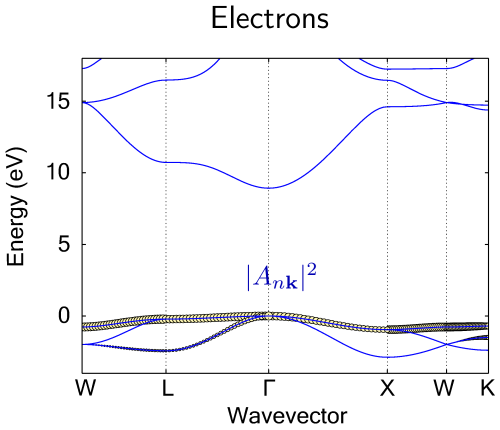
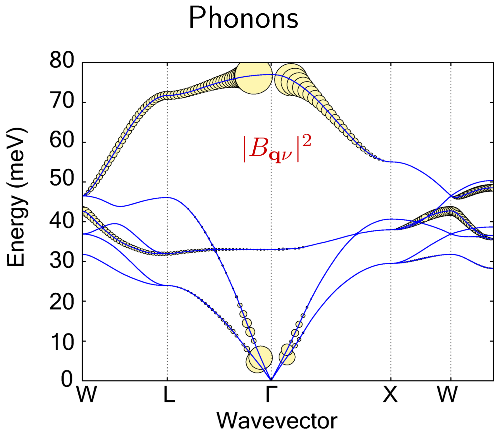
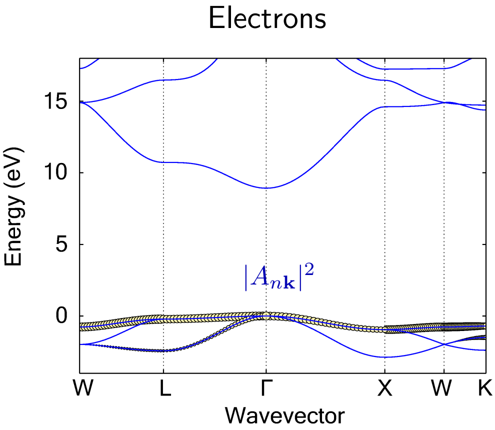
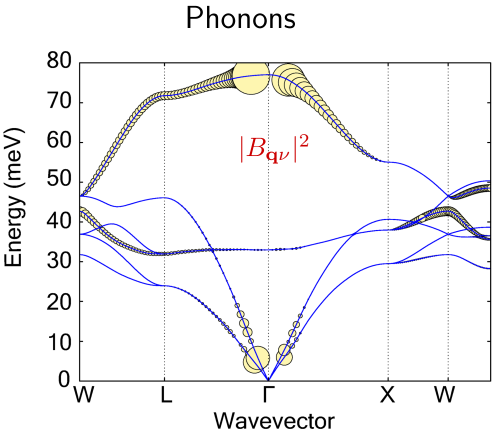


Figure from Sio et al, PRB 99, 235139 (2019)

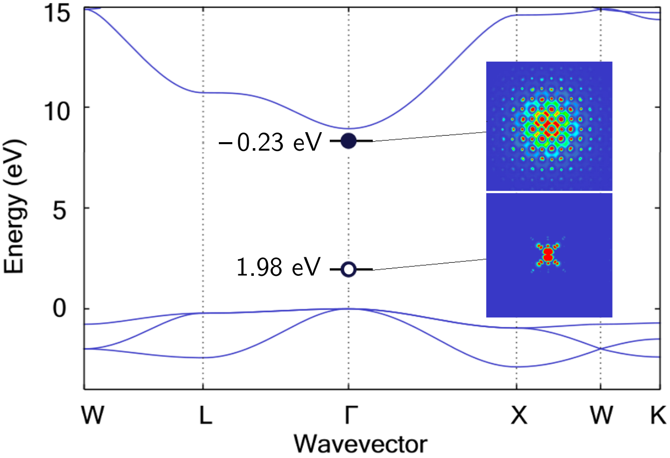

Electrons
Energy (eV)
15
10
5
0
$|A_{n\mathbf{k}}|^2$
W
L
Γ
X
W
K
Wavevector


Phonons
Energy (meV)
80
70
60
50
40
30
20
10
0
$|B_{\mathbf{q}\nu}|^2$
W
L
Γ
X
W
Wavevector





Holstein polaron



Shown are QP energies, eg $E_{N+1} - E_N$

Effect of self-interaction: A lesson from the Landau-Pekar model

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

Effect of self-interaction: A lesson from the Landau-Pekar model

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

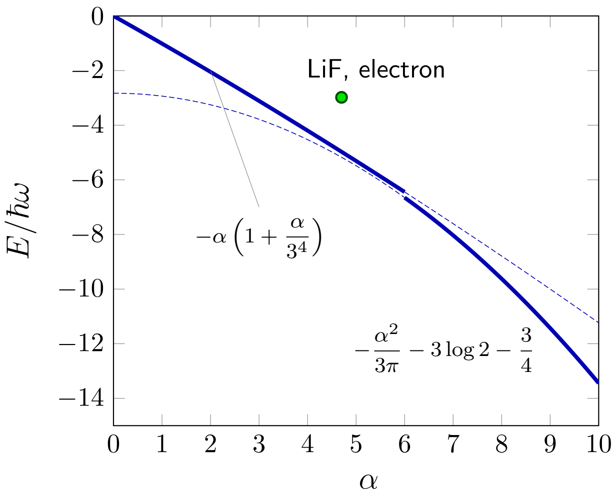
Effect of self-interaction: A lesson from the Landau-Pekar model

$$\hat{H}_{\mathrm{LP}} = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} \;+\; \boxed{\frac{e^2}{4\pi\varepsilon_0}\int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}}$$

$$\hat{H}_{\mathrm{LP}} = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\underbrace{\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} - 1\right)}_{[-1,0)}\int d\mathbf{r}'\,\frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}$$

- Hartree self-interaction suppresses localization
- Hybrid functionals partly cancel self-interaction

Formation energy vs. coupling strength*

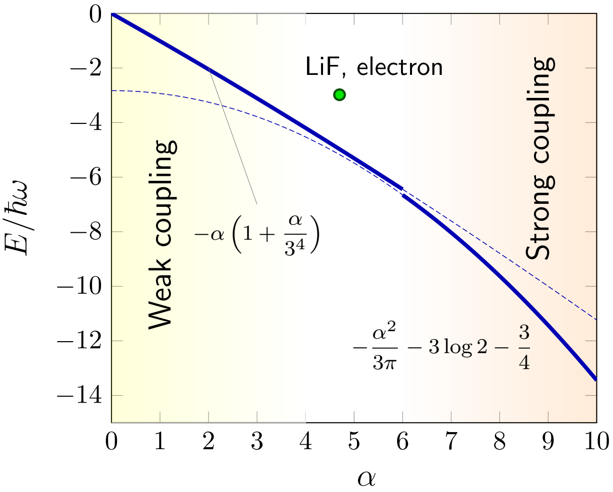


Similar to DMC results by Mishchenko et al, Phys. Rev. B 62, 6317 (2000)

*Valid only for Fröhlich model

From: Feynman and Hibbs, p. 318

Formation energy vs. coupling strength*



Similar to DMC results by Mishchenko et al, Phys. Rev. B 62, 6317 (2000)

*Valid only for Fröhlich model

From: Feynman and Hibbs, p. 318

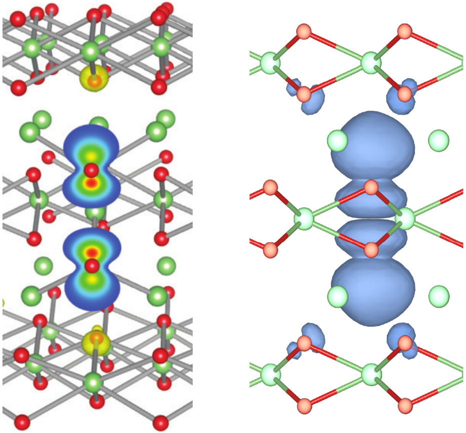
Take-home messages

- Many-body approach provides spectral function of polarons, but no wavefunction
- DFPT approach provides wavefunction of polaron, but no spectral function
- Progress in the study of polarons in real materials will likely require a combination of these approaches

References

- Franchini et al, Nat. Rev. Mater. 2021 [link]
- Devreese et al, Rep. Prog. Phys. 72, 066501 (2009) [link]
- Devreese, arXiv:1611.06122 (2020) [link]
- FG, Rev. Mod. Phys. 89, 015003 (2017) [link]
- Sio et al, Phys. Rev. Lett. 122, 246403 (2019) [link]
- Verdi et al, Nat. Commun. 8, 15769 (2017) [link]
- Nery et al, Phys. Rev. B 97 (2018) [link]
- Lee et al, arXiv:2011.03620 (2020) [link]

Perturbation approach vs. hybdrid DFT: Li_2O_2



Left figure from Feng et al, PRB 88, 184302 (2013); Right figure from Sio et al, PRL 122, 246403 (2019)