Artificial graphene as a designer Dirac material

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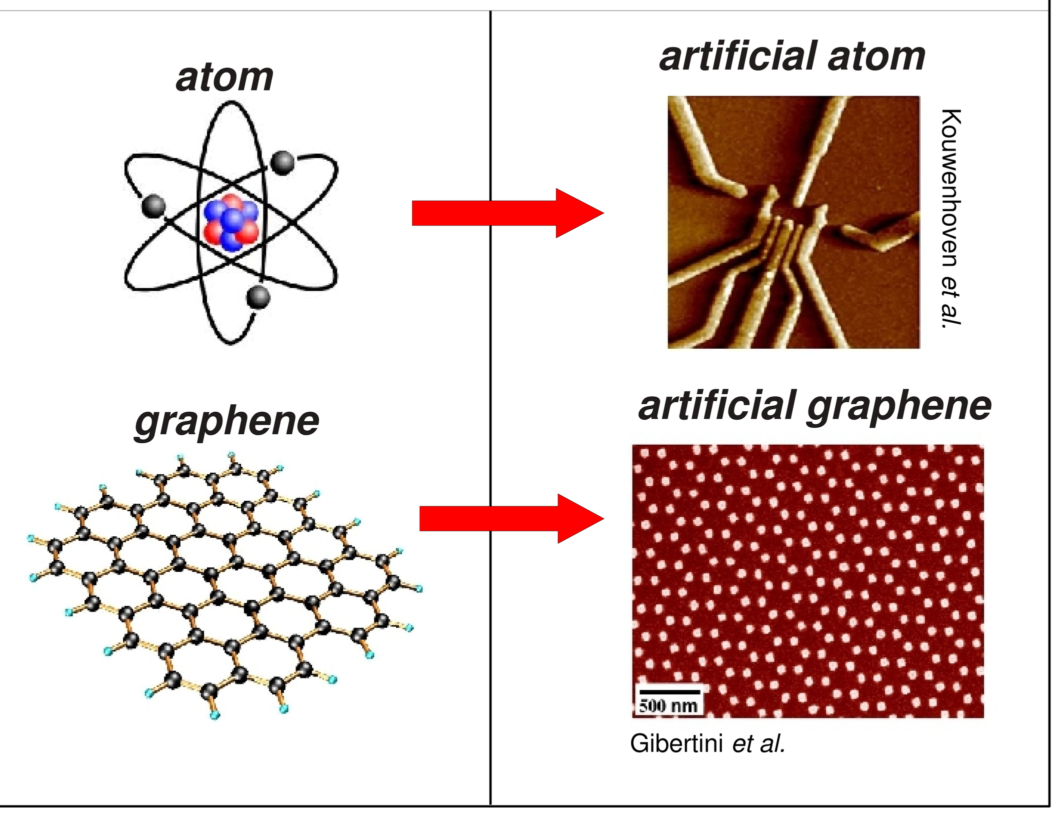
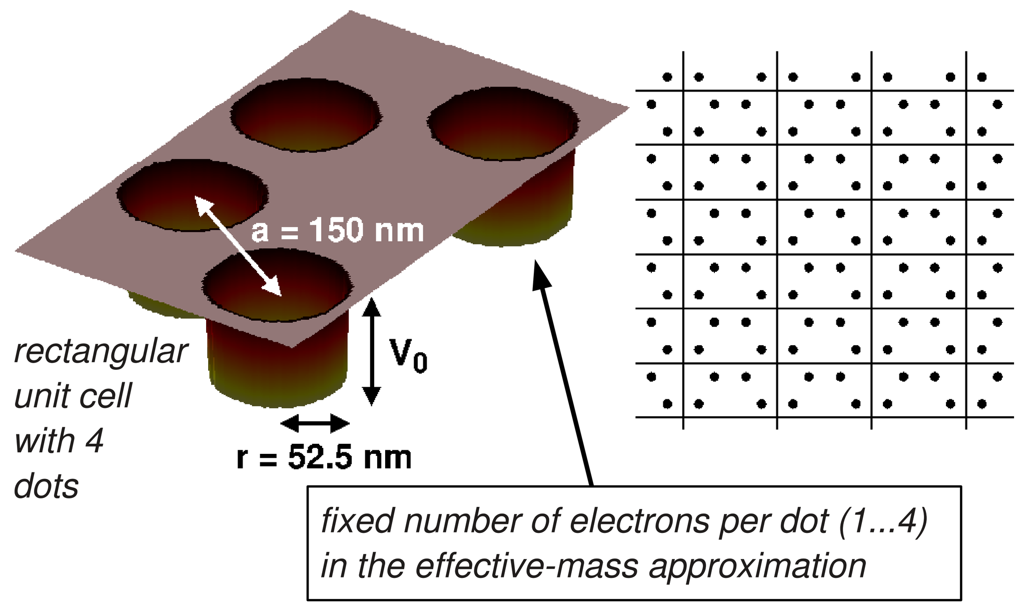
Main concept



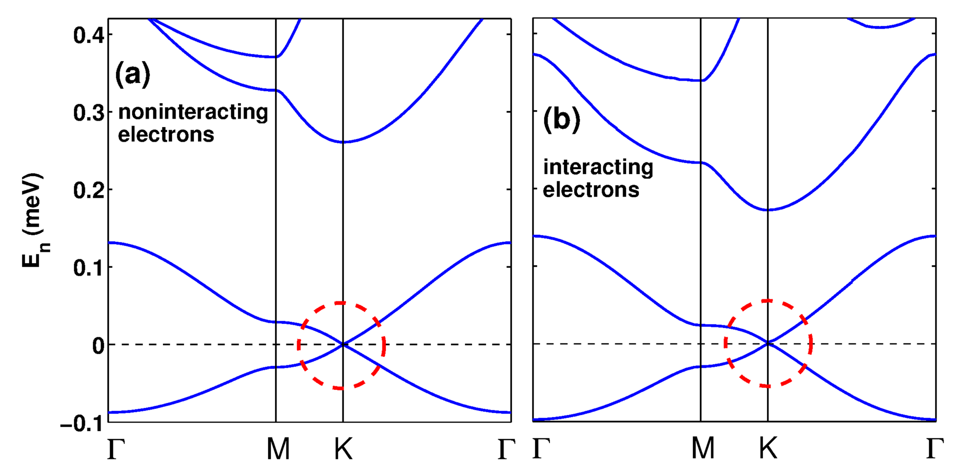
Real-space modeling (GaAs)

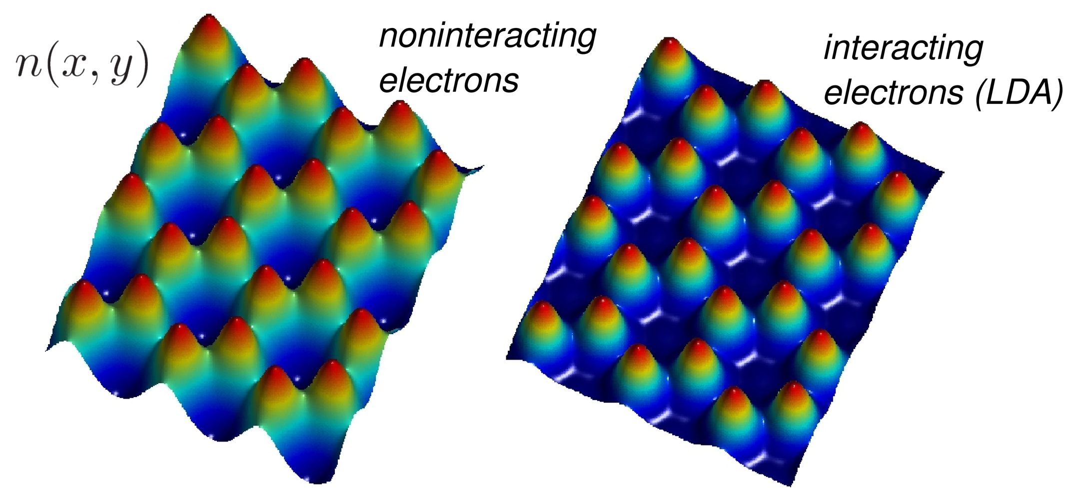


- Hard-wall model for the confining potential
- Real-space calculations in a periodic 2D system
- Electron-electron interactions dealt with DFT (see below)

Results

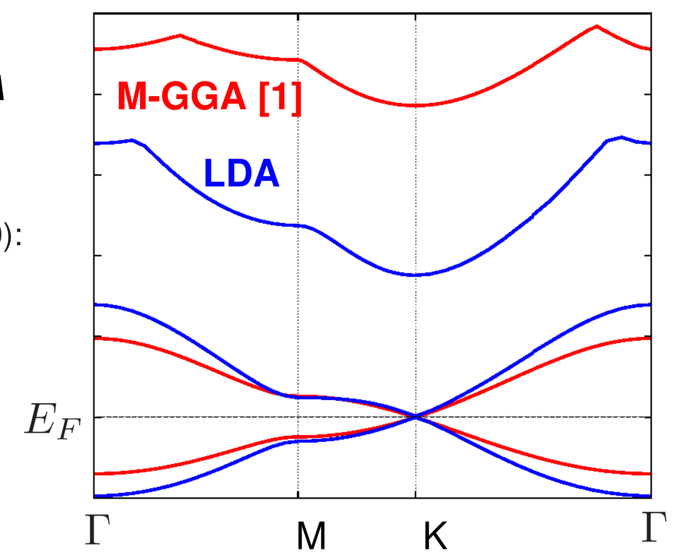
(1) one electron per dot: noninteracting vs. DFT (2D-LDA)





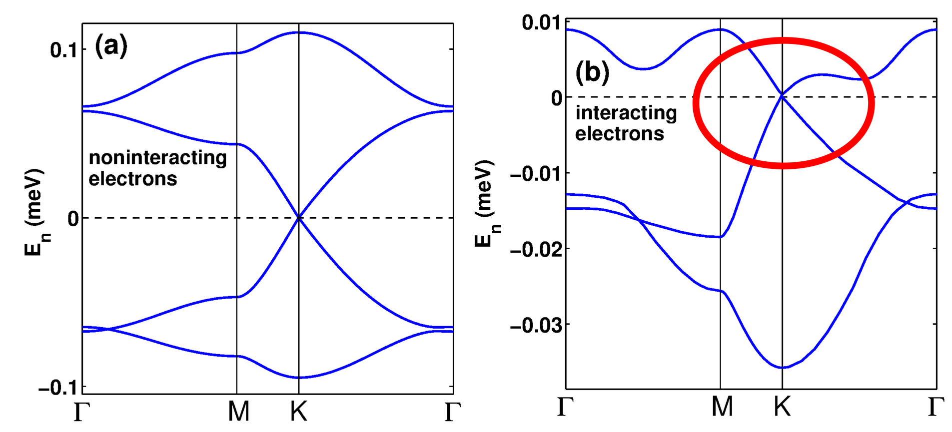
(2) one electron per dot: LDA vs. M-GGA

[1] M-GGA in PRB **81**, 115108 (2010): *correct asymptotic description of the electronic exchange*



Recent result from UPV/EHU San Sebastian (F. Berardi, A. Rubio et al.), ongoing collaboration

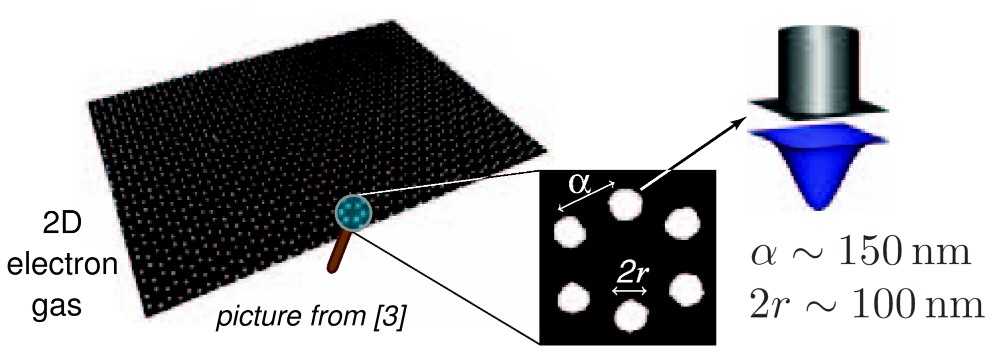
(3) four electrons per dot: noninteracting vs. DFT (2D-LDA)



- Dirac point relatively unstable in the presence of *intradot* electron-electron interactions

Experimental realization

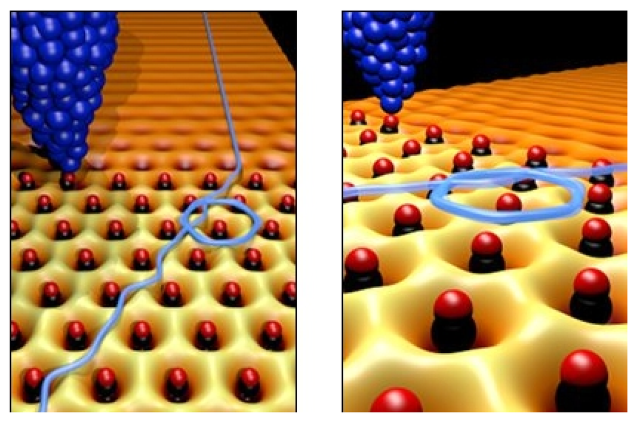
(1) Nanopatterned 2D electron gas (GaAs quantum well)



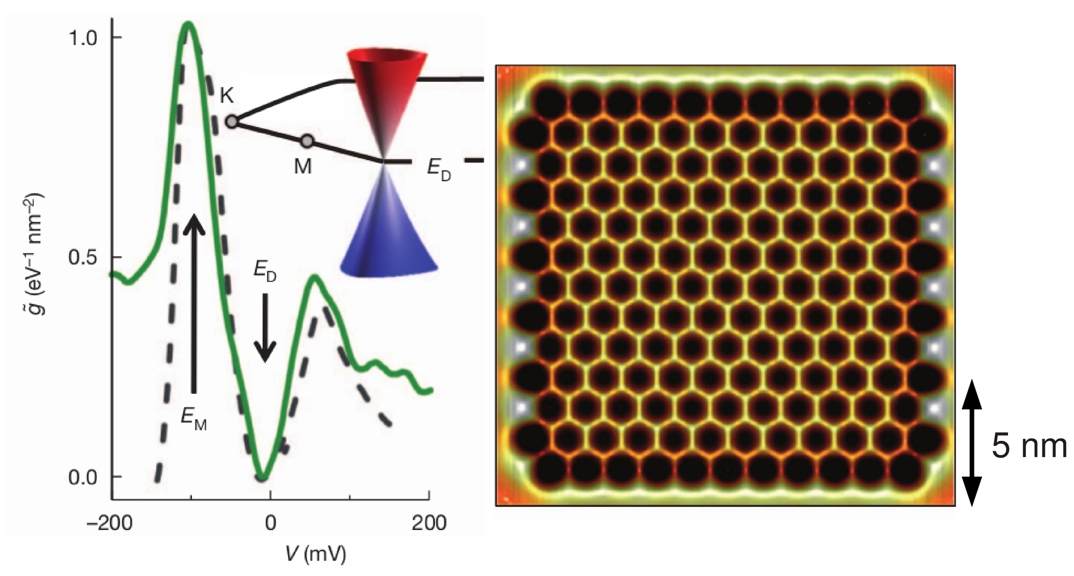
Idea:	[1] C.-H. Park and S. G. Louie, Nano Lett. **9**, 1793 (2009)
Realization:	[2] M. Gibertini *et al.*, Phys. Rev. B **79**, 241406(R) (2009)
Mott physics:	[3] A. Singha *et al.*, Science **332**, 1176 (2011)

- Photoluminescence & inelastic light scattering experiments; tight-binding calculations; demonstration of Mott-Hubbard physics
- Challenges: lattice homogeneity, distortion, coherence, interdot coupling

(2) Molecular graphene (CO molecules on Cu surface)



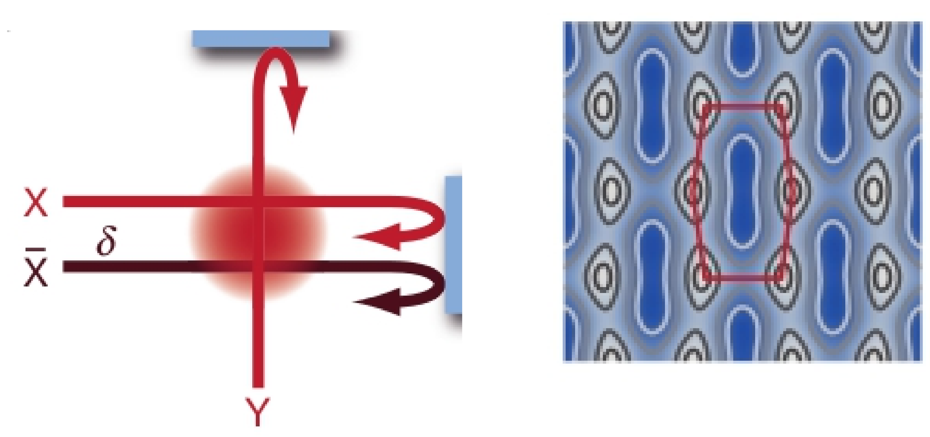
H. Manoharan / Stanford university



Gomes, Mar, Ko, Guinea, and Manoharan, Nature **483**, 306 (2012)

- Demonstration of Dirac point formation in surface-state conductance
- Additional experiments: p-n-p junction, Kekulé distortion, magnetic-field effects...

(3) "Optical graphene"

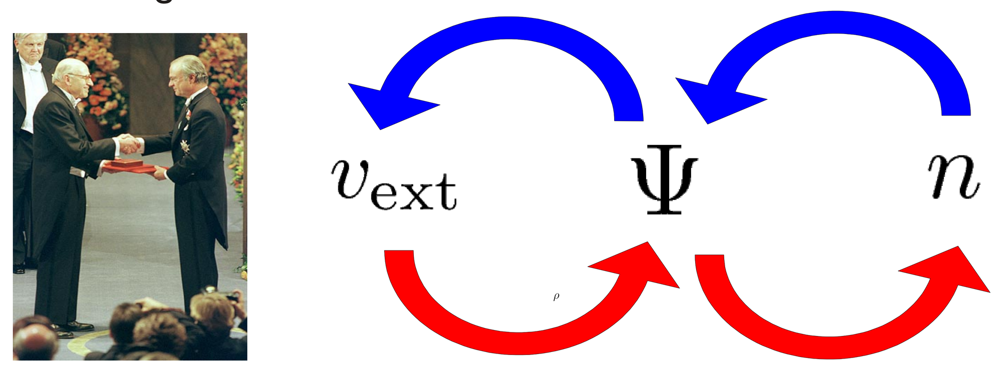


- Ultracold atoms in a honeycomb optical lattice

Tarruell, Greif, Uehlinger, Jotzu, and Esslinger, Nature **483**, 302 (2012)

Density-functional theory (DFT)

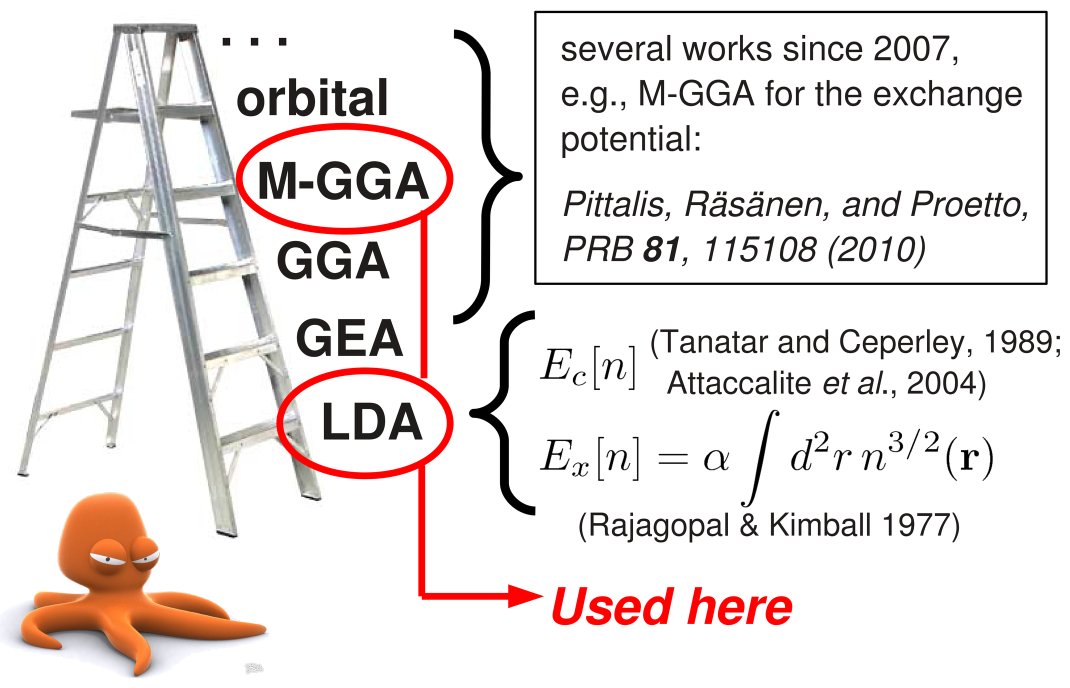
- Hohenberg-Kohn I:



- Hohenberg-Kohn II: $E[n_{\mathrm{GS}}] \leq E[n_{\mathrm{any}}]$
- Kohn-Sham: φ_i under $v_{\mathrm{eff}} = v_{\mathrm{ext}} + v_H + v_{xc}$ lead to n_{GS}

Density functionals for exchange and correlation

- "Jacob's ladder" of functionals available for 2D systems:

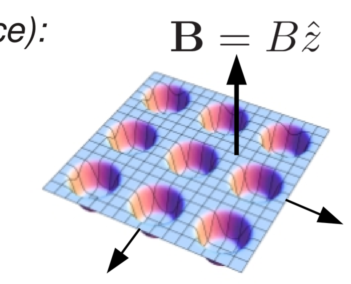


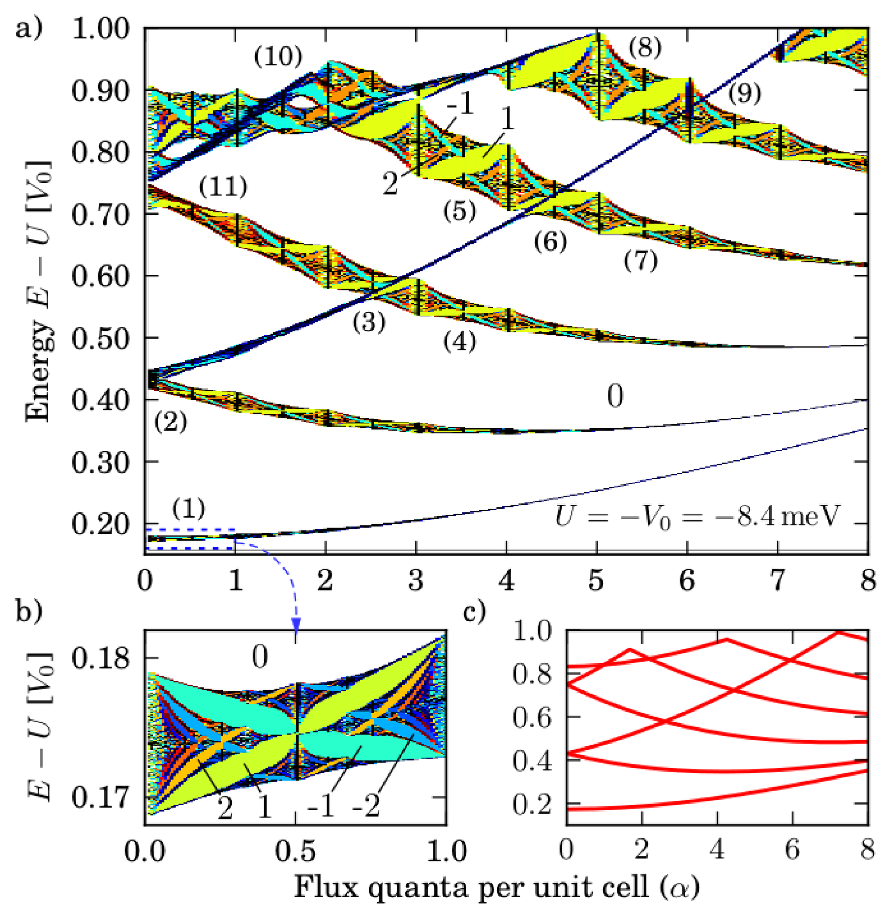
OCTOPUS code (GPL), *www.tddft.org*

Magnetic fields (work in progress)

(1) Finite systems (artificial graphene flakes):
=> straightforward inclusion of the vector potential (symm. gauge)

(2) Periodic systems (infinite honeycomb lattice):
=> generalized Bloch theorem in a magnetic unit cell + real-space solver for the Schrödinger eq., see Janecek *et al.*, arXiv: 1303.2020 with a square-lattice "Hofstadter butterfly" example (also below)





S. Janecek, M. Aichinger, and E. R. Hernández, arXiv: 1303.2020 (2013)

Summary and outlook

- Artificial graphene-like systems may lead the way into "designer Dirac materials"
- Artificial graphene experimentally demonstrated in 2009 - 2012 in quantum-dot lattices [1], metal surfaces [2], and optical lattices [3]
- Artificial graphene shows the Dirac point with linear dispersion as in real graphene [1,4]
- Density-functional calculations for quantum-dot artificial graphene show that the Dirac point is stable only at low population [4]
- Present / future projects: testing of different functionals, effects of distortion, magnetic-field effects / quantum Hall regime, modeling of different setups (molecular graphene), optical properties, coherent control, ...

[1] M. Gibertini *et al.*, Phys. Rev. B **79**, 241406(R) (2009)
[2] K. K. Gomes *et al.*, Nature **483**, 306 (2012)
[3] L. Tarruell *et al.*, Nature **483**, 302 (2012)
[4] E. Räsänen *et al.*, Phys. Rev. Lett. **108**, 246803 (2012)

Acknowledgments

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