

Table Ronde SFP@150 Les Grandes Questions Ouvertes et Enjeux Fondamentaux de la Physique'

> Antoine Georges Juillet 2023

Quantum Matter: Keys to Success



The magic Square

Materials Science and Chemistry New materials, bulk or `artificial' High quality samples New elaboration methods Theory Simple concepts and basic mechanisms Quantitative methods

Devices and Control Nanoscale devices e.g gating Atomic-scale synthesis e.g. oxide MBE `Synthetic materials' e.g. TBLG/Twisted TMOs Control by light: Laser control, Cavities,...

Materials Discovery

(A never-ending story that keeps us alive and busy)

- Classic correlated materials: TMs, Oxides/TMOs
- Organic conductors (1D, 2D)
- Heavy fermions
- Cuprates
- Renewal of interest in TMOs: Sr₂RuO₄, RNiO₃, Manganites, Iridates, and many many others...
- Mott to superfluid transition of cold atomic gases in optical lattices
- Topological Insulators
- Oxide heterostructures, SC in LAO/STO
- Fe-based superconductors
 - → `Hund metals' (New route to strong correlations)
- SC in pressurized H₂S 155GPa \rightarrow other hydrides
- SC in twisted bilayer graphene
- Twisted TMDCs
- \rightarrow Interplay of correlations and topology/Flat bands
- → Strong coupling to light, excitonic physics
 - SC in infinite-layer RNiO₂
 - Low density metals (STO), kagome metals



Timeline of Superconductor Discoveries (Wikipedia)



Novel Materials - `Semi-synthetic' - Devices **Novel forms of Quantum Matter:** - Cold atoms in optical lattices - Arrays of trapped Rydberg atoms OXIDES: Old and New



Rust: oxyde/hydroxide. (wikipe

 $La_{2-x}Sr_{x}CuO_{4}$

« Artificial materials » MBE allows for synthesis one atomic layer at a time



Example: Measurement of Electronic Compressibility

Article

Cascade of phase transitions and Dirac revivals in magic-angle graphene

https://doi.org/10.1038/s41586-020-2373-y Received: 25 November 2019 U. Zondiner¹⁵, A. Rozen¹⁵, D. Rodan-Legrain²⁵, Y. Cao², R. Queiroz¹, T. Taniguchi³, K. Watanabe³, Y. Oreg¹, F. von Oppen⁴, Ady Stern¹, E. Berg¹, P. Jarillo-Herrero^{2⊠} & S. Ilani¹¹





`Twistronics'



Image courtesy Pablo Jarillo-Herrero

REVIEW ARTICLE

https://doi.org/10.1038/s41567-020-01154-3

Check for updates

Moiré heterostructures as a condensed-matter quantum simulator

nature physics

Dante M. Kennes ^{1,2,12} , Martin Claassen ^{3,4,12}, Lede Xian ^{2,5,12}, Antoine Georges^{3,6,7,8}, Andrew J. Millis^{3,9}, James Hone ¹⁰, Cory R. Dean⁹, D. N. Basov ⁹, Abhay N. Pasupathy ⁹ and Angel Rubio ^{2,3,11}



Lattice	Model	Possible materials realizations	Correlated phases	
Twisted heterostructures of weakly correlated van der Waals monolayers				
Honeycomb	Two-orbital extended Hubbard model ¹⁸ ; fragile topological insulator ¹⁰⁷	TBG (BN substrate, with/without twist)	Mott insulation ⁸ ; superconductivity ⁷ ; correlated QAH insulator ^{22,23}	
	Two-orbital extended Hubbard model	Twisted double bilayer graphene	Ferromagnetic insulator superconductivity ^{12,13} ; triplet pairing ¹⁰⁸	
	Asymmetric $p_x - p_y$ Hubbard model ^{29,30}	Twisted bilayer MoS ₂ , MoSe ₂	Nematic (anti)ferromagnets ²⁹	
	Domain wall networks	Small-angle TBG with domain reconstruction 57,58,66,109		
Triangular	Hubbard model (with/without strong SOC)	Twisted bilayer WS ₂ , WSe ₂ (ref. ³⁴); twisted WS ₂ /WSe ₂ heterostructures ^{35,36} ; twisted double bilayers of WSe ₂ (ref. ¹¹⁰)	Correlated insulator ³⁴ ; superconductivity?; Wigner crystals ³⁵	
	Doped multi-orbital Hubbard models	Twisted heterostructures of MoS_{2} , WS_{2} , WSe_{2}	Moiré excitons ^{100,101,111}	
	Multi-orbital Kanamori models	Twisted bilayer BN	SDW; <i>d</i> -wave superconductivity ³²	
Rectangular	1D ionic Hubbard model 1D-2D crossover	Twisted bilayer GeSe	Luttinger liquid; Mott insulator; bond density waves ⁴³	
	Inverted band insulator, strong SOC	Twisted bilayer WTe_2	Quantum spin Hall insulator, fractional Chern/topological insulator	
Any	Hofstaedter models	TBG or TMDs in strong magnetic fields	Fractional Chern insulator ¹¹²	
Kagome	Kagome Heisenberg model	TBD	Z_2 QSL; U(1) QSL; quantum chiral spin liquid; valence bond crystal	
Decorated kagome	Hubbard model (putative)	Twisted bilayer MoS ₂ , MoSe ₂	TBD	
3D	Flat-band Hubbard-Kanamori models	Twisted multilayer 'staircase'	TBD	
Proximity effects				
Honeycomb, triangular	Proximity-induced Rashba SOC	TBG on WS ₂ , WSe ₂ substrate ¹¹³	Correlated QSH insulator	
Rectangular	Proximity-induced superconductivity	Superconductor, twisted bilayer GeSe, TMD 'sandwich' heterostructure	1D Kitaev superconductor; Majorana bound states	
Twisted heterostructures of correlated monolayers				
	Moiré ferromagnet ⁷⁰	Twisted odd-multilayer Crl ₃	Moiré domain wall; ferromagnets	
	Moiré Kitaev model	Twisted multilayer $\alpha\text{-}RuCl_3$	Kitaev QSL; stripe order; Majorana fermions	
	TBD	Twisted bilayer TaSe ₂	TBD	
	TBD	Twisted bilayer NbSe ₂	TBD	

Table 1 | Overview of possible quantum Hamiltonians, materials realizations and phases in twisted moiré heterostructures

TBD, to be discovered; QSL, quantum spin liquid; SOC, spin-orbit coupling.

Crystals of Light and Atoms: cold atomic gases in optical lattices



At the frontier of condensed matter physics and quantum optics...



Two novel routes to Control



Artificial Materials: Strained films and Heterostructures "Oxytronics/Mottronics"

Selective control with LIGHT



CONTROL: Traditional and Novel routes

Bandwidth	Pressure Size of rare-earth Distortion Tolerance factor 3d,4d,5d metal	
Crystal field, Orbital degeneracy	Size of rare-earth Distortion Tolerance factor	- Same -
Filling of shell	Chemistry	Ionic liquids Gating
Doping	Sr,Ca²+ → La, R ³+	
Interaction strength	3d,4d,5d metal	Tunable dielectric gating ? Light ?
Charge-Transfer	Change apical oxygen distance Change ligand: $O \rightarrow S, Se$	Light ?

Applied Physics Reviews

Cavity quantum materials o

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F. Schlawin,^{1,2} (D. M. Kennes,^{1,3} () and M. A. Sentef^{1,a} (



What About Theory?

- Up to the late 1980's our understanding of strong correlations was quite poor...
- Huge progress in 30 year!
- The raise of computational methods: theorists now have a right and a left hand (analytical/numerical)!
- Currently: very exciting times/recent developments in computational methods
- Merging of quantum many-body methods with realistic electronic structure → theory can be realistic (at last!)

Paul Dirac, 1929``Quantum Mechanicsof Many-Electron Systems' '

``The general theory of quantum mechanics is now almost complete (...).
The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, <u>and the difficulty is only that</u> <u>the exact application of these laws</u>

leads to equations much too complicated to be soluble."

P. A. M. Dirac, "Quantum Mechanics of Many-Electron Systems", Proceedings of the Royal Society of London, Series A, Vol.123, April 1929, pp 714.



 $H\Psi(r_1,\cdots,r_N) = E\Psi(r_1,\cdots,r_N)$

Eigenstates (wave-functions) and Eigenvalues (Energy spectrum)

Dirac's program' (same 1929 article):



``It therefore becomes desirable that <u>approximate practical methods</u> of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation."

Dirac's program is not yet fully implemented but great progress is being made → we can hope that this will be a major success of the 21st century! [Note that ``without too much computation" has an entirely different meaning now than in the 1930's ©]

Computational Methods: Handshake!

T/t

Temperature





Looking Immediately Ahead:

- Flat band physics
- Interplay of topology and correlations?
- Twisted layered oxides
- Light/Cavity control
- Finalize understanding of `simple' models
- Pushing the combination of electronic structure + many body methods to the next step: predictive/design
- Can we reach predictive ability for e..g superconductivity in strongly correlated materials

Two Big Challenges for the 21st Century

 The Dirac program: computational solution of the `quantum many body problem'

Materials by Design (Solid-State and Molecules)