# Let’s do it on a lattice!!!!

- Sandro’s invitation to work with him to develop an alternative way of doing Diffusion Monte Carlo (start of my PhD project in 2001): **invention of the Lattice Regularized Diffusion Monte Carlo (LRDMC)**

PRL 95, 100201 (2005) PHYSICAL REVIEW LETTERS week ending 2 SEPTEMBER 2005

**Diffusion Monte Carlo Method with Lattice Regularization**

Michele Casula,[1,2] Claudia Filippi,[3] and Sandro Sorella[1,2]

- **Quest for efficiency and accuracy** (the goal: being more accurate than DFT to solve first-principles Hamiltonians, by keeping the same efficiency)

# From lattice models to realistic systems

- Sandro's inspirational approach of "translating" his QMC developments for solving lattice models to *ab initio* Hamiltonians
- Source of inspiration for the whole *ab initio* community:

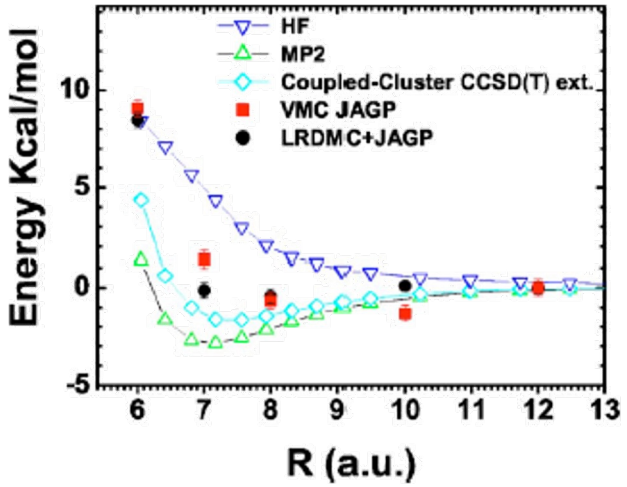
# From lattice models to realistic systems

- Sandro's inspirational approach of "translating" his QMC developments for solving lattice models to *ab initio* Hamiltonians
- Source of inspiration for the whole *ab initio* community:
  - ***New wave functions (Jastrow correlated Antisymmetrized Geminal Power)***
  - ***New optimizers (the stochastic reconfiguration method)*** *to minimize the variational energy with thousands of parameters*
  - *Geometry optimization via* ***efficient calculations of ionic forces in QMC (phonon calculations and molecular dynamics driven by QMC)***

# The quest for the “best” variational state: Jastrow correlated Antisymmetrized Geminal Power

- New ansatz for the *ab initio* problem with strong correlation:
  Jastrow correlated Antisymmetrized Geminal Power,
  extension of the Resonating Valence Bond wave function **(RVB)**.
  This gives the name to his QMC code: **TurboRVB**

# The quest for the “best” variational state: Jastrow correlated Antisymmetrized Geminal Power




**Weak binding between two aromatic rings: Feeling the van der Waals attraction by quantum Monte Carlo methods**

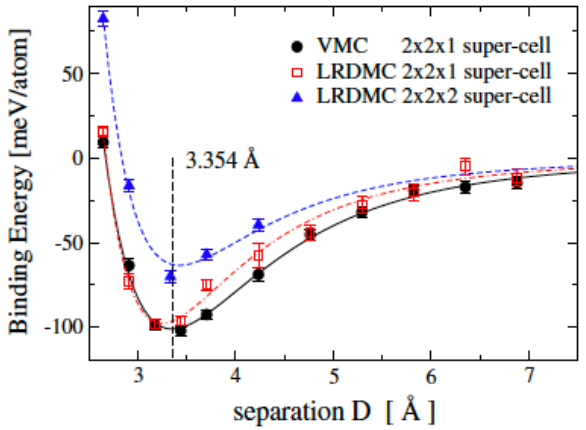
Cite as: J. Chem. Phys. **127**, 014105 (2007); https://doi.org/10.1063/1.2746035
Submitted: 05 February 2007 • Accepted: 09 May 2007 • Published Online: 02 July 2007

**Sandro Sorella, Michele Casula and Dario Rocca**

PRL **103**, 196401 (2009) PHYSICAL REVIEW LETTERS week ending 6 NOVEMBER 2009

**Nature and Strength of Interlayer Binding in Graphite**

Leonardo Spanu,[1] Sandro Sorella,[2] and Giulia Galli[1]

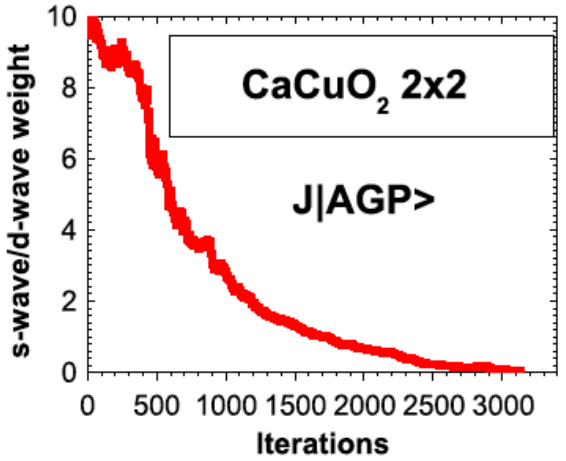


# The quest for the “best” variational state: Jastrow correlated Antisymmetrized Geminal Power

PRL 107, 086807 (2011) PHYSICAL REVIEW LETTERS week ending 19 AUGUST 2011

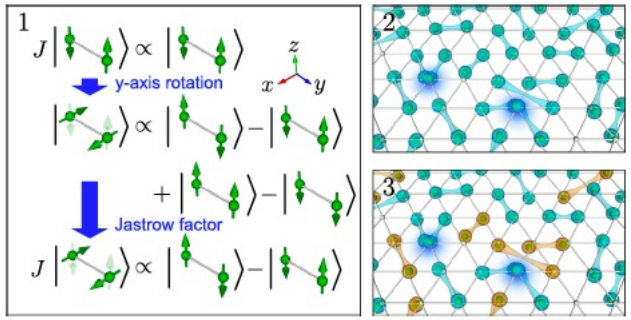
**Fate of the Resonating Valence Bond in Graphene**

Marchi, Azadi, Sorella




**Pairing symmetry in cuprates and iron-based superconductors entirely determined from first principles!**

**New paradigm for the chemical bond by using Pfaffians: covalent bond + spin fluctuations**






**The nature of the chemical bond in the dicarbon molecule**

Cite as: J. Chem. Phys. 153, 164301 (2020); https://doi.org/10.1063/5.0023067
Submitted: 26 July 2020 • Accepted: 04 October 2020 • Published Online: 22 October 2020

Claudio Genovese and Sandro Sorella

# Ionic force calculations in QMC

**Computing ionic forces with low variance and high efficiency (order $N^3$) in a QMC framework**

**Algorithmic differentiation and the calculation of forces by quantum Monte Carlo**

Cite as: J. Chem. Phys. 133, 234111 (2010); https://doi.org/10.1063/1.3516208
Submitted: 03 August 2010 • Accepted: 25 October 2010 • Published Online: 20 December 2010

Sandro Sorella and Luca Capriotti

**QMC-driven molecular dynamics and QMC phonon calculations made possible!**

PRL 100, 114501 (2008) PHYSICAL REVIEW LETTERS week ending 21 MARCH 2008

**Stable Liquid Hydrogen at High Pressure by a Novel *Ab Initio* Molecular-Dynamics Calculation**

Claudio Attaccalite[1] and Sandro Sorella[2]

PHYSICAL REVIEW B 103, L121110 (2021)

Letter Editors' Suggestion

**Atomic forces by quantum Monte Carlo: Application to phonon dispersion calculations**

Kousuke Nakano,[1,2,*] Tommaso Morresi,[3] Michele Casula,[3] Ryo Maezono,[2] and Sandro Sorella[1,†]

JCTC Journal of Chemical Theory and Computation Article
pubs.acs.org/JCTC

**Fully Quantum Description of the Zundel Ion: Combining Variational Quantum Monte Carlo with Path Integral Langevin Dynamics**

***Ab initio* molecular dynamics simulation of liquid water by quantum Monte Carlo**

Cite as: J. Chem. Phys. 142, 144111 (2015); https://doi.org/10.1063/1.4917171
Submitted: 10 December 2014 • Accepted: 27 March 2015 • Published Online: 14 April 2015

# Sandro’s legacy