The research activity involved the theoretical study of intermolecular forces, analytical developments within the DFT applied to model systems, multiconfigurational calculations in the context of VB and MO theories, some study of reactivity in solution and of solvation, calculations on boron and carbon clusters including nanotubes and graphitic structures and development and application of QMC in theoretical chemistry. In the context of the theory of intermolecular forces I have contributed (with R.McWeeny) to develop new ab initio methodologies within a matrix partitioning approach. Applications have been done on various systems and intermolecular potentials have been derived. Within the electron density theory, with N. H. March (Oxford-UK), several works have been done in order to relate all types of density functions of a fermion particle model system to the confining potential. With A. Nagy (Debrecen-HU), the attention has been moved to two body effects and pair density function. In the context of multiconfigurational calculations, I have focussed the attention on the transcription of a CASSCF wavefunction in terms of valence bond configurations. Application have been performed on a variety of systems including reacting systems on a reaction path in a complex environment. Within the theory of solvation, with B. Mennucci (Pisa-I), a new method for the calculation of the dispersion and Pauli repulsion contributions to the free energy of solvation has been proposed. This method is now implemented on the public version of the GAMESS-US package. About studies on boron and carbon clusters, various works have been done in collaboration with the group of N. H. March at the department of physics of the university of Antwerp (B). We have studied the intermolecular forces between two parallel C nanotubes, the solvation of fullerene in some organic solvents, the quantum network model applied to graphitic structures, some polarizability bound in C cages, the Thomas-Fermi and related models applied to C and B cages and tubes. Finally, in the field of quantum Monte Carlo, a scientific collaboration has been done with C. Filippi (NL). Work has been published on application of QMC to the theory of solvation (also with Floris-I), to the evaluation of correlated electron density for small systems and to the construction of new Jastrow-Slater wave functions based on localized orbitals for both ground and excited states. Actually, the research work is mainly addressed to the study of electron correlation in all aspects.

Schools and conferences attended since 2005 by Claudio Amovilli

1. Summer School and Miniconference on Dynamical Mean Field Theory, Trieste ICTP (Italy), 2005.
2. International Symposium on the Jahn-Teller Effects: Novel Aspects in Orbital Physics and Vibronic Dynamics of Molecules and Crystals, Trieste ICTP (Italy), 2006.
3. Advances in continuum quantum Monte Carlo methods, Cecam workshop, Lyon (France), 2007.
4. Advanced School in Quantum Monte Carlo Methods in Physics and Chemistry, Trieste ICTP (Italy), 2008.
5. Graphene Week 2008, Trieste ICTP (Italy), 2008.
   Poster: C. Amovilli, N. H. March, F. E. Leys, I. A. Howard, A. Rubio, D. J. Klein, F. M. Floris, "Graphitic structures: network models, C cages properties and solvation of fullerene".
6. Quantum Monte Carlo in the Apuan Alps VI, Vallico Sotto (LU), Italy,2010.
   Invited Talk: C. Amovilli, "Chemistry of nitrosamine: a QMC study of the thermal de-NOx process" and "Quantum Monte Carlo formulation of volume polarization in dielectric continuum theory".
7. Psi-K Conference 2010, Berlin (D), 2010.
8. DFT-11 Conference 2011, Athens (GR), 2011.
9. The VIII Congress of the International Society for Theoretical Chemical Physics (ISTCP-VIII), Budapest (HU), 2013.
   Poster: C. Amovilli, F. Fracchia, C. Filippi, "Size-extensive wave functions for QMC: The J-LGVBn theory".
   Poster: F. M. Floris, C. Filippi, C. Amovilli, "A Polarizable Continuum Model of solvation designed for QMC: ground and excited states of solutes".
10. The "March" meeting. A symposium in honor of Norman H. March, Namur (B), 2013.
    Poster: C. Amovilli, "The Quantum Monte Carlo method: at the frontier of computation".
11. International Conference: Smart functional materials for shaping our future, Debrecen (HU), 2014.
    Invited Talk: C. Amovilli, "Potential energy surfaces with Quantum Monte Carlo".
    Poster: F. M. Floris, R. Guareschi, C. Filippi, C. Amovilli, "Excited states of molecular solutes with Quantum Monte Carlo(QMC): vertical transition and geometry optimization".
12. 16th International Conference on Density Functional Theory and its Applications, Debrecen (HU), 2015. Poster: C. Amovilli, F. M. Floris, A. Grisafi, "Localized polycentric orbital basis set for Quantum Monte Carlo calculations derived from the decomposition of Kohn-Sham optimized orbitals".
13. The 8th Molecular Quantum Mechanics, June 26 - July 1, Uppsala, Sweden, 2016.
    Poster: C. Amovilli, F. M. Floris, "A novel continuum model for the calculation of solute-solvent dispersion contribution to the electronic excitation energy in solution".
14. 17th International Conference on Density Functional Theory and its Applications, Tallberg (Sweden), 2017.
    Invited Talk: C. Amovilli, "Properties of electron density in weak binding conditions".
    Poster: F. M. Floris, C. Amovilli, "Shannon entropy and correlation energy for electrons in atoms".
15. Strasbourg satellite meeting to the 16th ICQC: Strong correlation in electronic structure theory, June 24-27, Strasbourg, France, 2018.
    Poster: C. Amovilli, F. M. Floris, "Critical conditions (zero ionization potential) in model N_2-like molecular ions".
16. The 9th Molecular Quantum Mechanics, June 30 - July 5, Heidelberg, Germany, 2019.
    Poster: C. Naim, E. Ramos-Cordoba, E. Matito, C. Amovilli, "Analysis of nondynamic electron

correlation in DFT".
Poster: F. M. Floris, C. Amovilli, "Intermolecular Pauli repulsion: a QMC study of molecules in an excited state in free space and in solution".

Short term visits (C. Amovilli)

1. Institut de Quimica Computational, University of Girona, (Spain), September 1999.
2. Department of physics, University of Antwerp (Belgium), February 2002.
3. Department of physics, University of Antwerp (Belgium), December 2003.
4. Condensed Matter Research, Trieste ICTP (Italy), August 2004.
5. Instituut-Lorentz for Theoretical Physics, Universiteit Leiden (NL), March 2006.
6. Instituut-Lorentz for Theoretical Physics, Universiteit Leiden (NL), April 2007.
7. Department of Theoretical Physics, University of Debrecen (HU), December 2007.
8. Department of Theoretical Physics, University of Debrecen (HU), May 2008.
9. Instituut-Lorentz for Theoretical Physics, Universiteit Leiden (NL), February 2009.
10. Department of Theoretical Physics, University of Debrecen (HU), May 2009.
11. Faculty of Science and Technology, University of Twente (NL), February 2013.
12. Department of Theoretical Physics, University of Debrecen (HU), September 2013.

Research Projects (C. Amovilli):

1. 1999-now, University of Pisa, Theoretical Chemistry, Fondi di Ateneo, PI
2. PRIN 2000, National, participant
3. PRIN 2004, National, participant
4. PRIN 2006, National, participant
5. PRIN 2009, National, PI of Pisa Research Unit
6. 2006-9, CNR (Italy) - MTA (Hungary) joint project, Pair density functional theory, Italian PI
7. CINECA-ISCRA Class C Project (HP10C9066L) 2010, PI
8. TÁMOP-4.2.3 project (2012, Hungary, EU), Smart Material, participant
9. PRA_2016_46, University of Pisa, Study of Confined Systems: towards a Multiscale Approach, PI
10. PRA_2018_36, University of Pisa, Chirality in Chemistry: a Holistic Approach, participant