

## SCIENTIFIC ACTIVITY OF LORENZO RESCA

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Since the mid 1980's, I have been mostly interested and contributed to five different areas of research: (A) Electronic structure of semiconductor heterostructures and superlattices; (B) Electrical response in heterogeneous systems and electrorheological fluids; (C) First-principles theory of ferroelectricity; (D) Psychophysical measurements and computer simulations of eye movements in visual search; (E) Theory, computation, and engineering of thermoelectric materials.

With regard to the first area (A), mainly in collaboration with R. D. Graft, M. Fornari, D. J. Lohrmann, and G. Pastori Parravicini, we have applied recursion-renormalization methods to study the microscopic structure of heterostructures and superlattices. We have studied in particular HgCdTe quantum wells and superlattices, with technological applications to infrared detectors. Accurate microscopic wavefunctions have been obtained, allowing a more detailed study of interface states, semiconductor-semimetal transitions, and valence-band offset. We have also applied Green's function and recursion methods to study localized defects and impurities in semiconductors, demonstrating relative contributions of Coulomb tails, central cell potential, and intervalley interference, resulting in a "shallow-deep instability" that has been subsequently found and demonstrated in many other systems. Previously, we had used quantum defect methods to study excitons in rare-gas and other molecular solids, including fullerenes.

With regard to the second area (B), mainly in collaboration with L. Fu, we have developed an analytical method to calculate exactly the classical electrical response of heterogeneous systems. Our method is based on a multipolar re-expansion, and includes all the multipolar images generated in the experimental configuration of parallel electrode plates, as well as in other substrate configurations. We also applied this multipolar method to the mean field theory of disordered systems, including two-particle distributions of all multipolar orders. We studied in particular clusters of spheres and inclusions with permanent multipoles, solving problems of anomalous infrared absorption in composites and resolving ambiguities in the original models of Debye and Onsager. A major application of our multipolar method has been to electrorheological fluids (ERF), allowing to calculate exactly the electrostatic interactions and forces among the suspended particles, and between the particles and the electrodes. We have demonstrated rigorously that dipole approximations, often used in calculations and simulations, yields only a few percent of the exact forces at typical ERF densities. We have shown in particular that an ERF consisting of metal spheres coated with a thin insulating layer exhibits largely enhanced electrostatic forces. Another major application of our multipolar method has involved nonlinear composites. We have shown that the effective nonlinear (third order) susceptibility for disordered systems of coated spherical particles can be enhanced by five to seven orders of magnitude, and that the peak frequency can be largely shifted, through the combined effects of the particle structure and the inter-particle interactions. As a result, the

nonlinear spectrum can be sensitively tuned by varying a given concentration-distribution parameter. We have extended our theory to all ranges of applied fields, producing both the weak- and strong-field nonlinearities as particular limits. Striking and unexpected results have been found at intermediate fields, consisting of multiple solutions in certain frequency ranges. This may still have major implications for optical communications and laser technologies.

With regard to the third area (C), mainly in collaboration with L. Fu, E. Yaschenko, and R. Resta, we have contributed to seminal research in the theory of ferroelectricity. Ferroelectric materials have unusual properties in their structural, electrical, and electromechanical behavior. Such properties stem from the electronic structure of these materials, where the highly variable hybridization of the relevant orbitals plays a critical role. We elucidated in particular the relationships between electronic levels, crystal structure, and electrical properties. Namely, we have explained underlying microscopic mechanisms, understood general trends, and interpreted various experiments. In dealing with these materials and properties, a quantum-mechanical first-principles approach is essential. Our approach has consisted in performing first-principles calculations using methods of modern electronic-structure theory and state-of-the-art technical ingredients. An important characteristic of our work has been the use of both Hartree-Fock and density-functional methods, which provide results having the same overall quality, but with errors typically providing opposite bounds to the experimental results. In another fundamental development, we have shown that the very fact that insulators have a finite bulk polarization originates from the essential localization of the electronic wavefunction. We have thus provided a novel definition of electronic localization, and demonstrated the value of this concept not only for “non-exotic” insulators, but even for a highly correlated model material. Furthermore, we have studied several surface properties of ferroelectric perovskites, and pointed out those properties —such as dynamical charges— where a naive extrapolation of the bulk results leads to even qualitatively incorrect values. Other inquiries of ours have delved into non-ferroelectric oxides, where we have predicted some unexpected polarization features. From the technological point of view, ferroelectric materials are currently used in the most effective acoustic transducers. Our research has contributed to an understanding at the fundamental level that fosters a more rational and systematic search of better materials for such transducers.

With regard to the fourth area (D), mainly in collaboration with T. D. Keech, we have conducted psychophysical measurements of eye movements in young and older adults performing conjunctive visual search tasks, and thus determined corresponding elements of perception, selection, attention, and memory. We have found age-related differences in various measures of eye movements, consistently indicating slightly reduced conspicuity areas for older adults —hence, correspondingly reduced processing and memory capacities. Most importantly, we have demonstrated the formation of spiraling or circulating patterns in the eye movement trajectories and developed a corresponding computational model and simulations. The relation of attention, memory and spatial constraints to pattern formation in eye movement trajectories has been demonstrated through studies of saccade autocorrelations and power spectra that confirm a bias to progress forwardly, while turning at the display boundaries, plus a long-range memory

component for the search path. Analyses of certain measures of circulation and imbalance in the eye trajectories, and their relations with the display area correspondingly subtended, also bear signatures of spiraling or circulating patterns. We have interpreted their prevalence as mainly due to the interactions between three basic psycho-neural mechanisms (conspicuity area, forward bias, long-range memory) and two task-specific geometric-spatial constraints on the eye trajectories (central start and display confinement). Conversely, computer simulations of random walks in which all psycho-neural mechanisms are eliminated, while geometric-spatial constraints are maintained, show no prevalence of circulating patterns by those measures. We did find certain peculiarities of some individual participants in their pattern selections, but they appear too casual and incidental to suggest more systematic or complex search strategies in our randomized displays of uninformative stimuli. Most notably, we have developed a computational model and corresponding computer simulations that mimic phenomenologically the eye movement trajectories observed in a conjunctive visual search task. The element of randomness is captured in the model through a Monte Carlo selection of a particular eye movement based on its probability, which depends on three factors, adjusted to match the observed saccade amplitude distribution, forward bias in consecutive saccades, and return rates. Memory is assumed to operate through tagging of objects already recognized as non-target, which in turn requires their processing within the attentional area of conspicuity (AC). That AC is adjusted so that computer simulations reproduce optimally the distribution of the number of saccades, the failure rate to capture the target, and the return rate to previously inspected locations. For their viability, computer simulations critically depend on memory to be long-ranged. In turn, the simulations confirm the formation of circulating or spiraling patterns in the observed eye trajectories. We have also related consistently the average number of saccades per trial to the saccade amplitude distribution by modeling analytically the combined roles of the AC in attention and memory.

With regard to the fifth area (E), mainly in collaboration with N. A. Mecholsky, I. L. Pegg and M. Fornari, we have developed a theory of angular effective mass and band structure warping to study electronic and thermal properties of materials, using first-principles calculations and computer simulations to apply and support it. That should guide the engineering of thermoelectric materials so to optimize their thermoelectric performance and transport properties. That includes subjecting materials to perturbations such as strain or doping, or fabricating them as heterostructures, superlattices, nanostructures or nanowires, thus tailoring their electronic band structures and warping to affect transport coefficients and figures of merit as optimally desired.

## **CURRICULUM VITAE OF LORENZO RESCA**

Date and place of birth:  
Born on June 1<sup>st</sup>, 1949, in Bologna, Italy.

Education:

- Laurea in Fisica (magna cum laude), Department of Physics, University of Pisa, 1970.
- Diploma di Licenza in Fisica della Scuola Normale Superiore (SNS) di Pisa, 1970.
- Master of Arts in Psychology, Catholic University of America, 2013.

#### Positions:

- SNS student fellow, 1966-1970.
- National Research Council (CNR) postdoctoral fellow, Department of Physics, University of Pisa, 1971-1973.
- CNR researcher, permanent appointment, Department of Physics, University of Pisa, 1974.
- Army engineer, second lieutenant, Military Academy of Cecchignola, Rome, 1975-1976.
- Research Associate, Department of Physics, Purdue University, West Lafayette, Indiana, 1977-1979.
- NATO Senior Fellow, 1980.
- Assistant Professor, Department of Physics, The Catholic University of America, Washington, D.C. 20064, 1980-1985.
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2. G. Pastori Parravicini and L. Resca, "Electronic states and optical properties in cubic ice", *Phys. Rev. B* 8, 3009 (1973).
3. L. A. Gomez, G. Pastori Parravicini, L. Resca, and R. Resta, "Valence bands and Davydov splittings in solid ortho-hydrogen", *J. Phys. C* 6, 1926 (1973).
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82. L. Resca, “Space-time and spatial geodesic orbits in Schwarzschild Geometry”, submitted to *European Journal of Physics*.

## TEACHING AT THE CATHOLIC UNIVERSITY OF AMERICA

I have taught all the core courses of both the undergraduate and graduate curriculum, plus numerous advanced courses on continuum mechanics, chaotic dynamics, quantum field theory, many-body theory, relativity and cosmology. For all of these courses, I have prepared and provided to the students extensive and detailed notes, problems, and solutions. A partial list of courses that I have taught at CUA since 1980 follows:

- PHYS 215 (4) University Physics I, S(pring)81, F(all)83.  
 PHYS 216 (4 Credit Hours) University Physics II, S84, S89.  
 PHYS 611 (4) Math. Meth. Theoretical Phys. I, F81, F82, F01.  
 PHYS 612 (4) Math. Meth. II, S82, S83, S84, S95, S99, S01, S04, S07, S11.  
 PHYS 615 (3) Adv. Mechanics I, F80, F81, F84, F95, F97, F99, F01.  
 PHYS 616 (3) Adv. Mechanics II, S81, S82, S83, S91, S93, S02.  
 PHYS 616 (3) Adv. Mech. II: Chaos in Dynamical Systems, S96, S05.  
 PHYS 618 (3) Continuum Mechanics, S96.  
 PHYS 621 (3) Stat. Mech. I, F89, F90, F93, F94, S96, S98, F00, F02, F04, F05, F06, F08.  
 PHYS 622 (3) Stat. Mech. II, S90, S91, S94, S95, F96, F98, S01, S03, S05, S06, S07, S09.  
 PHYS 623 (3) Advanced Electromagnetic Theory I, F85, F86, S88.  
 PHYS 624 (3) Adv. E&M Theory II, S86, S87, S90, S03, S04.  
 PHYS 659 (4) Adv. Quantum Theory I, F84, F91, F07, F16, F17.  
 PHYS 660 (4) Adv. Quantum Theory II, S85, S86, S92, S08, S17.  
 PHYS 665 (3) Solid State Physics I, F91, F11, F12.  
 PHYS 666 (3) Solid State Physics II, F92, F04, S12.  
 PHYS 725 (3) Advanced Classical Electrodynamics, F87, S89.  
 PHYS 740 (3) Quantum Th. of Many-Particle Systems, S93, F95, F97.  
 PHYS 750 (3) Theory of Relativity, S94, S99, F03, F09.  
 PHYS 751 (3) Gravitation and Cosmology, F99, S10.  
 PHYS 761 (3) Quantum Field Theory I, F86, S88, F93, F05.  
 PHYS 762 (3) Quantum Field Theory II, F94, S06.