After a stage in experimental Condensed Matter Physics during her Master Degree, Maurizia Palummo has worked in the field of ab initio calculations of the structural and electronic properties of materials. In particular during her Ph.D. she worked with Dr. Lucia Reining (Ecole Polytechnique, Palaiseau, France) performing pioneering GW calculations on wide-band gap materials. A member of the European Theoretical Spectroscopy Facility, she is an expert in the most modern theories and computational tools of ab initio electronic structure calculations (density functional theory and many-body perturbation theory methods). The main focus of her present research is on the calculation of electronic and optical properties of surfaces, organic molecules and derivatives and nanostructures, mainly nanowires and novel 2D/layered materials. She has been co-organizer of several international conferences and schools. In the last years she was a visiting scientist for several periods in the group of Prof. J. C. Grossman (MIT USA), Prof. M. Bernardi (Caltech USA) and Prof. K. Yamashita (Tokyo Univ., Japan).

She is author of more than 100 articles in international scientific journals, since 2017 she has been Associate Professor at the Physics Department of the University of Rome "Tor Vergata", Italy.