



METHODOLOGY		
General keyword	Details in topic	Researchers involved
DFT, large-scale, Second-Principles, SIESTA, Scale-Up	Development of the DFT code SIESTA	Javier Junquera, Pablo García-Fernández
	Development of the second-principles (first-principles-based) methods for large-scale simulations in materials	Pablo García-Fernández, Javier Junquera

APPLICATIONS			
Systems	Property	Methods	Researchers involved
Ferroelectrics and their interfaces	Negative compressibility, polarization, electric susceptibility, chirality, polarons	DFT and second-principles	Javier Junquera
			Pablo García-Fernández
Transition-metal containing solids	Optical and magnetic properties	DFT and second-principles	José Antonio Aramburu and Pablo García-Fernández