

METHODOLOGY			
General keyword	Details in topic	Researchers involved	Institute (Group Acronym)
<p>A: Software Development: Integration in our software (ASAP) of new module (Linux, shell scripting, Python, PyQt, Fortran, Git)</p>	DFT, SIESTA & ABINIT codes	Yann Pouillon / Peter Koval	<p>SIMUNE https://www.simuneatomistics.com/services-products/asap-software/</p>
	Electronic Transport - TRANSIESTA- ANT		
	Classical MD, LAMMPS code		
	Force Fields - Machine Learning		
	Image Recognition - Machine Learning		
Quantum Chemistry - Scattering theory - MOLCAS			

B: Project Execution (using one of our supported codes (ASAP, SIESTA,	ab-initio MD, MD, DFT, coarse-grained models		See examples of material / applications at https://www.simuneatomistics.com/case-studies

APPLICATIONS				
Systems	Property	Methods	Researchers involved	Institute (Group Acronym)
A: Increase the functionalities of our product				
B: Preparation of Scientific Material for Marketing (Case Studies / Slides & Movies)				