MS16-P09 | INVESTEGATION OF PHYSICAL PROPRIETIES OF EQUIATOMIC SILVER-RARE EARTH COMPOUNDS AG-RE (RE=ND, CE ,GD) FROM FIRST PRINCIPLES CALCULATIONS.

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Density functional theory (DFT) within generalized gradient approximation (GGA) pseudo-potentials and plane waves basis VASP (Vienna ab initio Software Package) are used to investigated physical properties of silver –rare earth equiatomic binary alloys Ag-Re (Re=Gd,Nd, Ce). Elastic proprieties have been computed and showed that these compounds have the strongest alloying ability and structural stability. A much better agreement was achieved between the Mechanical properties calculated results and the reported experimental data.