

Each participant randomly gets his metal (Na, K, Mg, Al, Ga, Ti, V, W )

- Level 1: Vacancy and self-interstitial formation energies
  - several possibilities for self-interstitial
  - compare with experiment and other calculations
- Level 2: Substitution/interstitial defects
  - look in literature to choose 3-5 reasonable solutes forming solid solutions
  - choose elements wisely to study relationships (solute lattice vs solution energy, solute radius vs solution energy, etc)
  - compare with experiment and other calculations

Each participant randomly gets his metal (Na, K, Mg, Al, Ga, Ti, V, W )

- Level 3: Defect complexes: vacancy-solute, vacancy-vacancy, interstitial-solute
  - calculate binding energies
  - compare to other calculations if any
- Level 4: Diffusion and self-diffusion
  - calculate vacancy migration barrier
  - calculate solute migration barrier
  - compare with experiment and other calculations if any