A picture containing text, screenshot, line, diagram

Description automatically generated

A->B

* What is dimensionality of compound name
* What is sample type of compound name in experiment
* What code is used for compound name in simulation
* What is formula of compound name
* What is group of compound name
* What is iupac of compound name

A->B+C

* What are organic and inorganic components for compound name

A->B->C

* What is experimental result of compound name in experiment

(experimental result refers to

synthesis starting materials

synthesis product

synthesis description

experimental method

experimental description)

* What is simulated result of compound name in simulation

(simulated result refers to

level of theory

Exchange-correlation functional

k-point grid

level of relativity

basis set definition

numerical accuracy)

Unable to answer

* What is sample type/experimental result of compound name in simulation
* What code is used for/ What is simulated result of compound name in experiment