

Active learning homework assignment with hands-on activities

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The following problems will help you better understand data querying and to modify workflows to fit your needs. Before starting with the assignment make sure you go over the accompanying lecture and hands-on tutorial. For the assignments below, you will work with the *Querying Data Repositories* notebook in the following tool: <https://nanohub.org/tools/matdatarepo>. You will need an API key to access data from Materials Project, follow the instructions in the tool.

Problem 1. Extend data query. Using information provided by the documentation page (<https://materialsproject.org/docs/api>), add piezoelectric properties to the query. Include an image of your dataframe showing your successful piezoelectric property query.

Problem 2. The default color scheme for the bulk modulus vs. shear modulus plot is in black scatter points. Add a new layer of dimension to your figure. Color code the scatter plot to correspond with the Poisson ratio.

Problem 3. Filter results for elasticity AND now for piezoelectric constants. Rather than coloring the shear vs. bulk modulus figure with Poisson's ratio, extract the appropriate data from the piezoelectric data to color code the plot using refractive index.

Problem 4. Using the code below, write an expression to query the Materials Project to create a new dataset with elasticity for every compound that has ever been calculated and published on the repository. Re-create the bulk vs. shear modulus figure and include it in your solution. Which compound has the highest bulk modulus, which has the highest shear modulus?

```
elastic_data = mpr.query({"elasticity": {"$exists": True}}, properties=[])
```