Create a project:

New project→enter BN_elastic→click the OK

Input crystal structure:

Import→Navigate to Structures\Semiconductors→double-click on BN.msi (grey: B, blue: N), which is a cubic phase of F-43M.

Optimize the Crystal Structure:

1. from the menu bar: Build→Symmetry→Primitive Cell
2. Module→Castep→Calculation
   Setup→ Task:Geometry Optimization; Quality: Fine; Functional: GGA and PW91
   Click More for the Geometry Optimization →Check the Optimize cell box→Run.
   After run, cell parameters of about a = b = c = 2.574 Å.

Calculate the elastic constants of BN

1. Module→Castep→Calculation
2. Setup→Task: Elastic Constants
3. Click More for the Elastic Constants dialog→Increase the Number of steps for each strain from 4 to 6→ close the dialog→Ensure that BN CASTEP GeomOpt/BN.xsd is the active document→Click the Run button.
4. After the run: Modules→CASTEP→Analysis→ Select the Elastic constants option→Ensure the results file from the Elastic Constants job to be displayed in the Results file selector→Click the Calculate button.
   A new text document, BN Elastic Constants.txt, is created in the results folder.

Description of the elastic constants file

Two strain patterns are required for this lattice type (F-43M).

For each strain pattern, there is a summary of calculated stresses as extracted from the respective .castep files.