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Calculation of elastic constants at high pressure from first-principles

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Elastic constants can be defined via either the energy-strain or stress-strain relationships. Although the formal theory is well established, their computation using the energy-strain relationship can lead to erroneous results at non-zero pressure. This talk discusses various corrective solutions that have been put forward to address this issue. An alternative method that is physically transparent and avoids the complexities of previous suggestions is then proposed.