

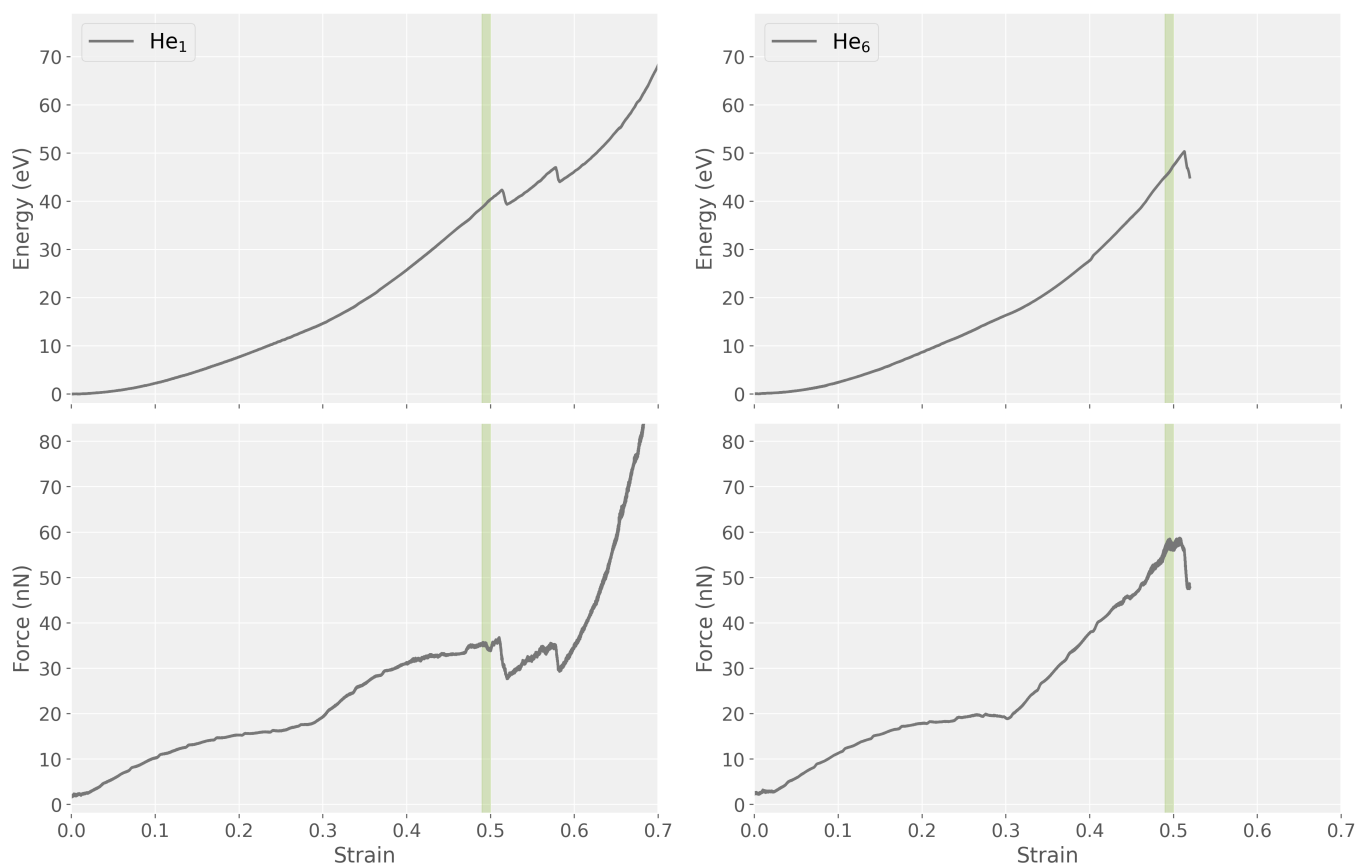
Supplemental Material: "First principles molecular dynamics calculations of the mechanical properties of endofullerenes containing noble gas atoms or small molecules"

Laurent Pizzagalli

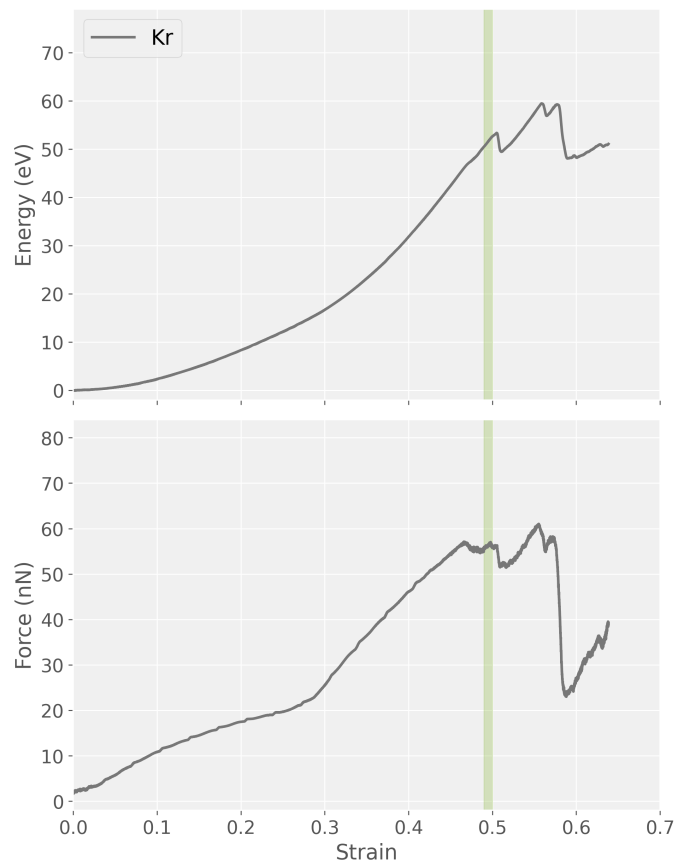
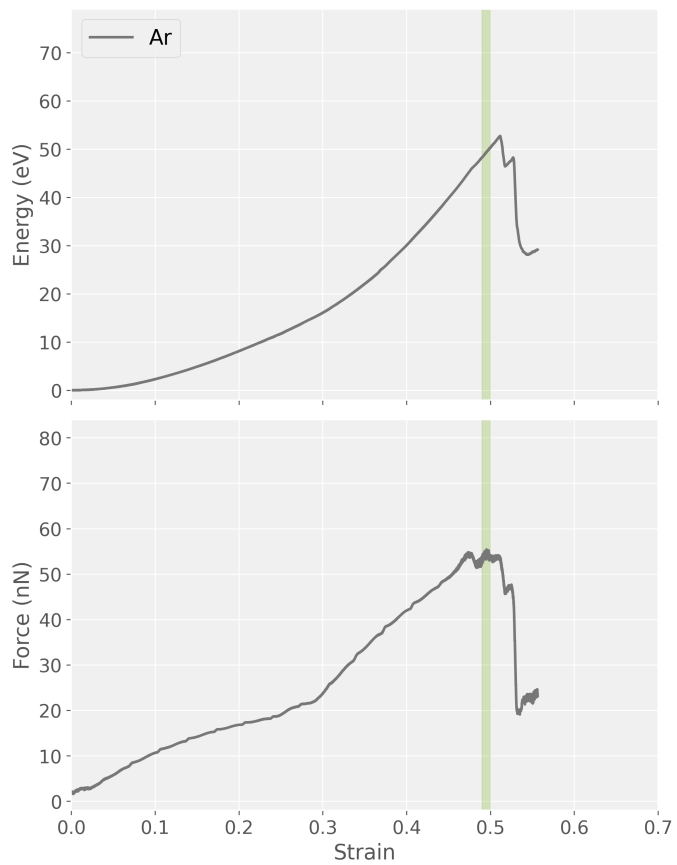
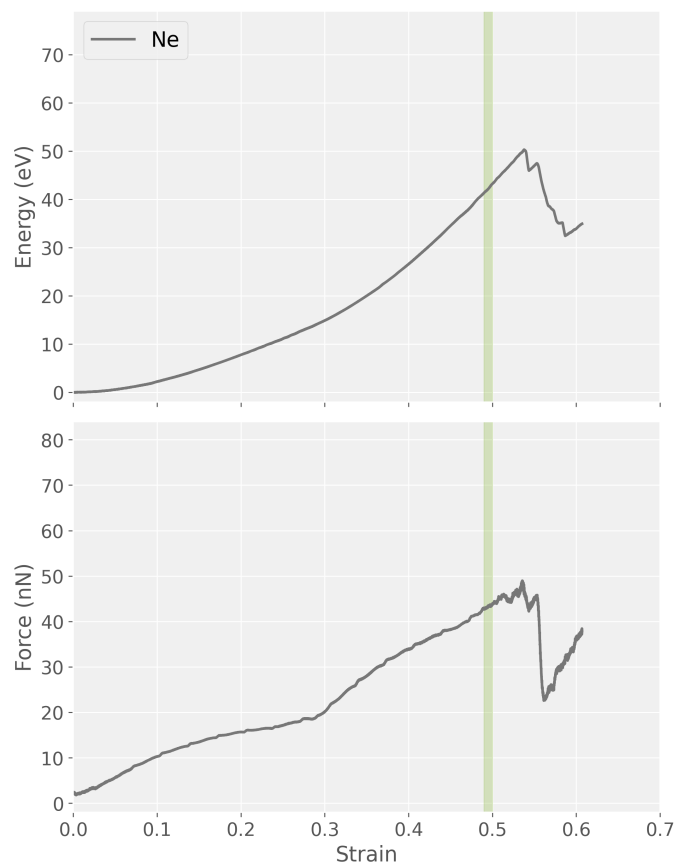
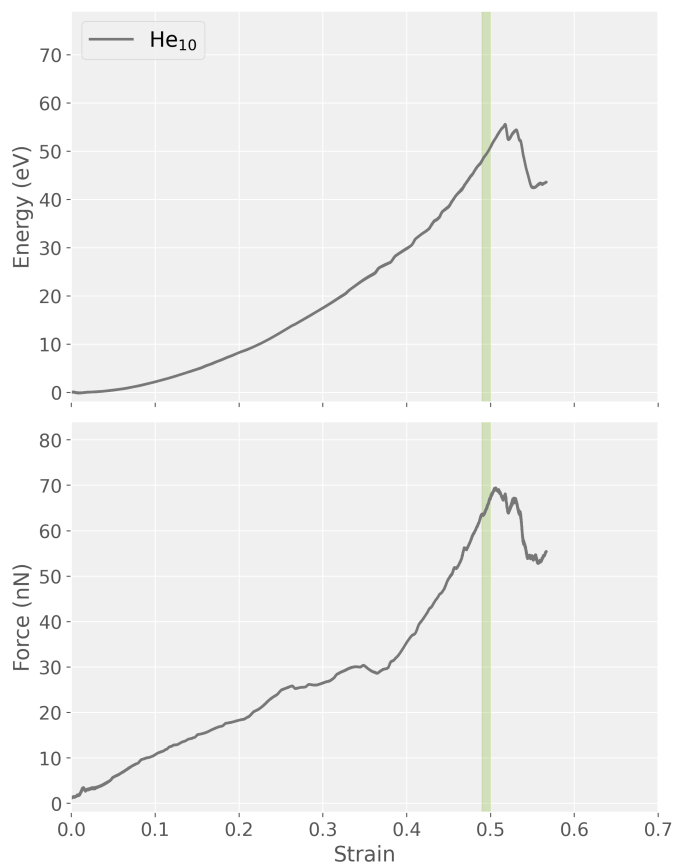
*Institut Pprime - CNRS UPR3346, Université de Poitiers, F86962 Chasseneuil Futuroscope Cedex, France**

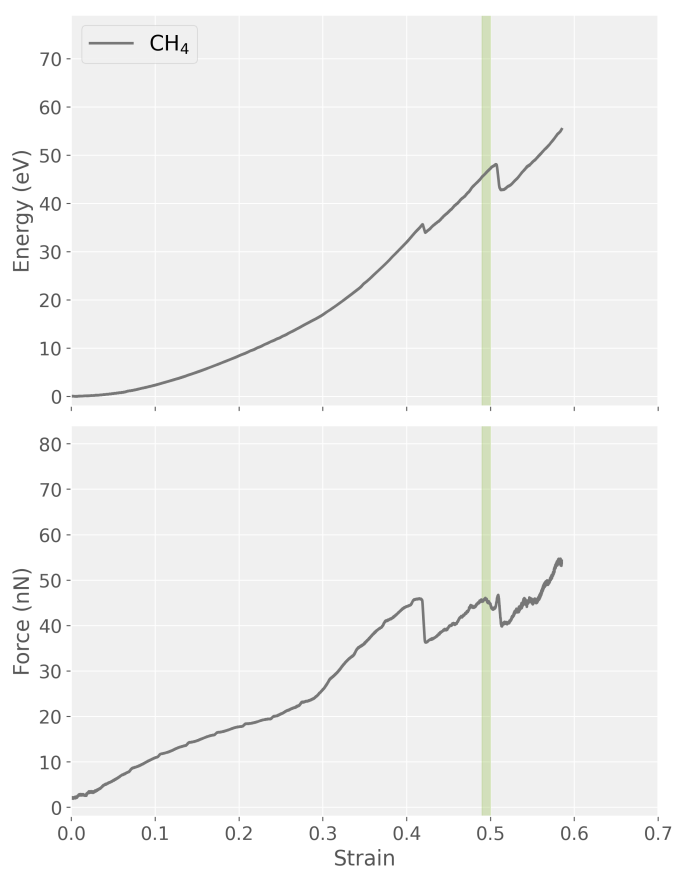
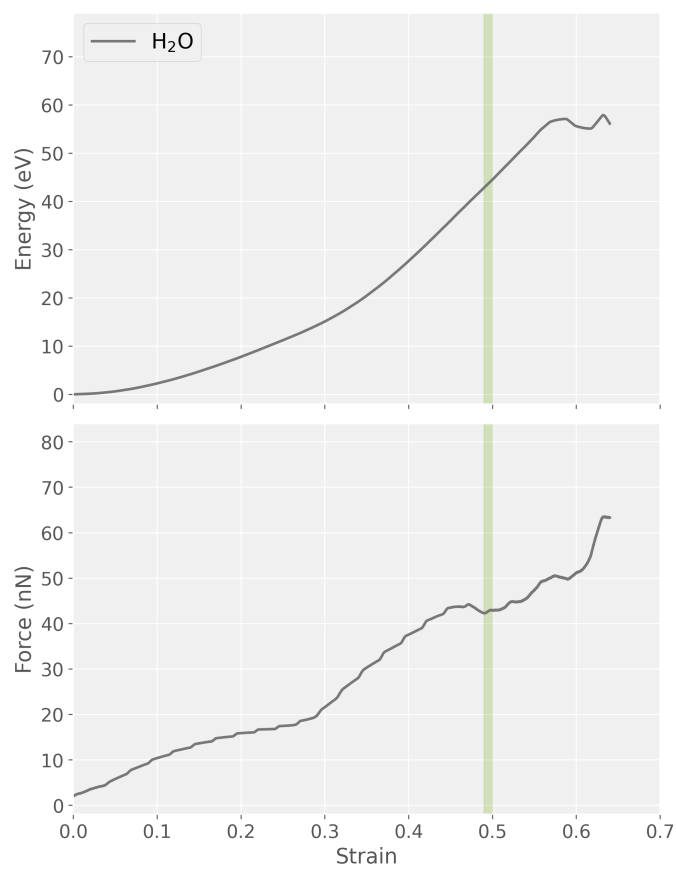
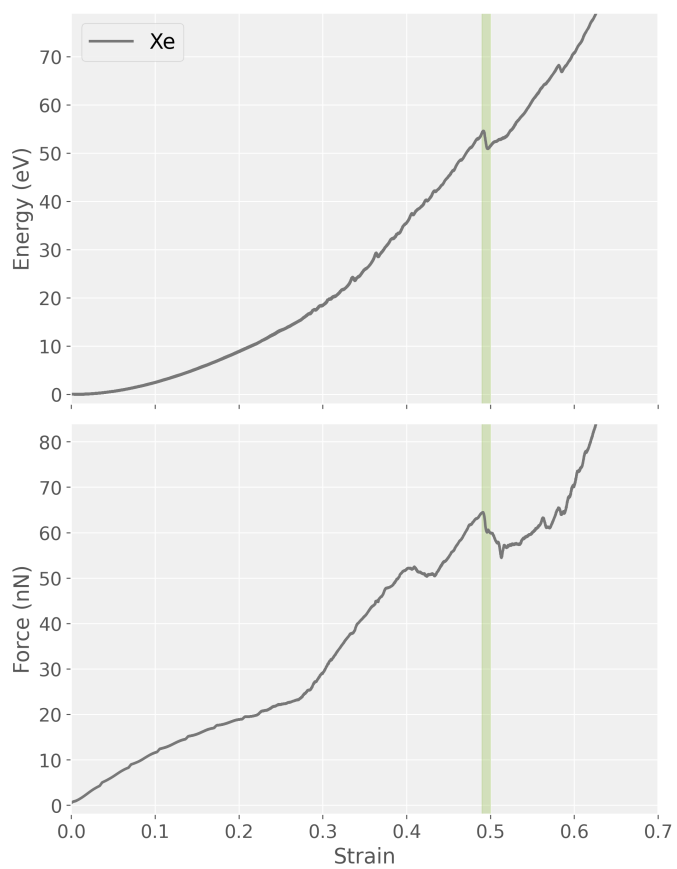
S1. ENERGY|FORCE VERSUS STRAIN

The graphs below show the variations of total energy and contact force computed during the compression of various endofullerenes.



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S2. MOVIES

The movies "*H2O@C60.mp4*" and "*CH4@C60.mp4*" show the structures of H₂O and CH₄ using ball-stick models during a uniaxial compression at 300 K.