DFT study of curvature effects in graphene flakes

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Curvature effects on mechanical and electronic properties of fixed size graphene hexagonal flakes are studied. Several values of spherical and pseudo-Taub NUT curvatures (figure 1) are applied to a hexagonal-shaped graphene flake generated with a tailor-made numerical software. A hybrid system of molecular mechanics optimizations and Density Functional Theory (DFT) single-point energy calculations is used to get the total energies and the spectra, from which the curvature energy and the gap are extracted. By plotting these results against the curvature parameter *k* an exponential relationship k^n is expected for both curvature energy and gap. This relationship is confirmed for the pseudo-Taub NUT function flakes, while for the spherical ones a slow change in the exponent *n* is observed (figure 2). This behaviour is further studied with a nonlinear extrapolation for larger radius, from which an asymptotic exponent of -2, compatible with available continuous models [1], is extracted.

REFERENCES

[1] ZHOU, Yanguang *et al.*, Carbon, 84 (2014) 263-271

FIGURES

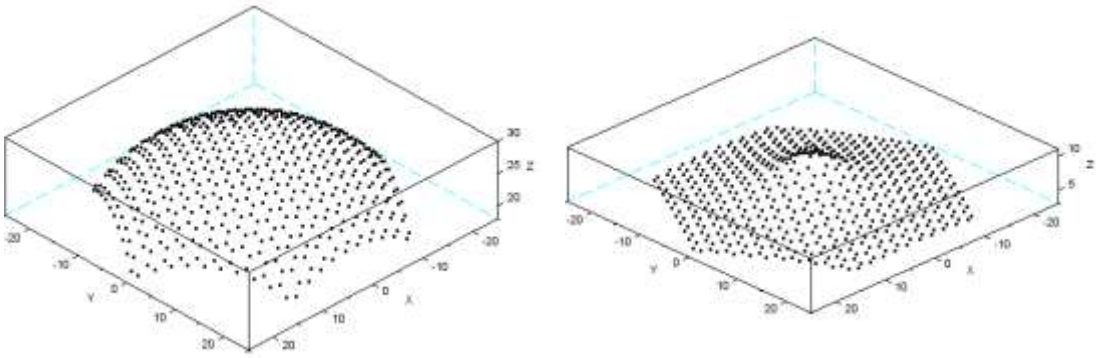

Figure 1: Examples of spherical (left) and pseudo-Taub NUT (right) curvatures in hexagonal graphene flakes.

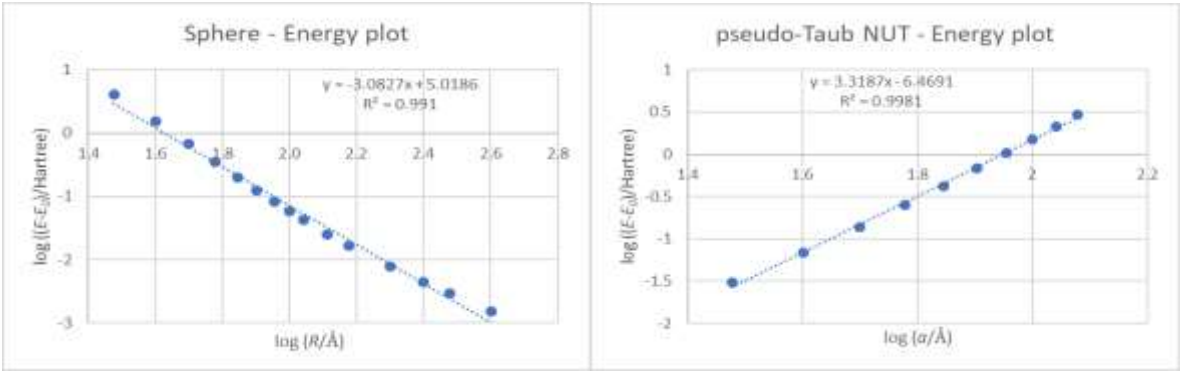

Figure 2: Energy plots for both curvatures studied, with least-squares fittings.