

Eight favorite papers of Humberto Terrones and why

**1.- Mackay, A.L. and Terrones, H., "Diamond from Graphite", *Nature*, Vol. 352, 762, (Aug. 1991).
DOI:10.1038/352762a0**

In this paper the concept of Negative Gaussian curvature was introduced theoretically to produce periodic sp^2 curved crystals. These structures were named Schwarzites after Hermann Amandus Schwarz also are called Mackay-Terrones crystals.

**2.- Terrones, H. and Mackay, A.L., "The Geometry of Hypothetical Curved Graphite Structures",
Carbon Vol. 30, No. 8, 1251-1260, (1992). DOI:10.1016/0008-6223(92)90066-6**

In this paper using differential geometry, different sp^2 carbon nanostructures are studied using changes in Gaussian curvature, Positive Gaussian curvature for Fullerenes, Negative Gaussian curvature for Schwarzites and zero Gaussian curvature for graphene. The curvature is introduced through "topological defects" such as pentagons, Heptagons, octagons, etc.

3.- Terrones, M., Terrones, H., Banhart, F., Charlier, J.-C., Ajayan, P.M., "Coalescence of Single-walled Carbon Nanotubes", *Science*, Vol. 288, No 5469, 1226-1229 (2000).

DOI: 10.1126/science.288.5469.1226

For the first time using high resolution transmission electron microscopy the coalescence of single walled carbon nanotubes were observed. A theoretical model involving vacancies and negative Gaussian curvature is involved in the coalescence. DOI: 10.1126/science.288.5469.1226

4.- Seifert, G., Terrones, H., Terrones, M., Jungnickel, G., Frauenheim, Th., "Structure and electronic properties of MoS_2 nanotubes", *Physical Review Letters*, Vol. 85, No 1, 146-149 (2000).

DOI: 10.1103/PhysRevLett.85.146

In this manuscript for the first time the electronic properties for nanotubes made of transition metal dichalcogenides (TMDs) were calculated, finding direct and indirect band gaps depending on their structure (arm-chair indirect gap zigzag direct gap). These results show the first theoretical evidence of direct band gap in single layer TMD.

5.- Terrones, H., Terrones, M., Hernández, E., Grobert, N., Charlier, J.-C. and Ajayan, P.M., "New metallic allotropes of planar and tubular carbon", *Physical Review Letters*, Vol. 84, No. 8, 1716-1719 (2000).

DOI: 10.1103/PhysRevLett.84.1716

In this manuscript different 2-Dimensional crystals of graphene are studied. The crystals exhibit a balance of positive (pentagons of carbon) and negative Gaussian curvature (heptagons of carbon). The structures are named Haeckelites in honor of Ernst Haeckel because the resemblance with the radiolaria drawings.

6.- Rodriguez-Manzo, Terrones, M., Terrones, H. , Sun, L., Banhart, F., Kroto, H.W., ``In situ nucleation of carbon nanotubes by the injection of carbon atoms into metals", *Nature Nanotechnology*, Vol. 2, 307-311 (2007).

DOI: [10.1038/nnano.2007.107](https://doi.org/10.1038/nnano.2007.107)

In this manuscript by using high resolution transmission electron microscopy the birth of a multiwalled and single walled carbon nanotubes is observed in-situ for the first time.

7.- Terrones, H., Lv, R., Terrones, M., Dresselhaus, M.S., ``The Role of defects and doping in 2-D graphene sheets and 1 D nanoribbons", *Reports on Progress in Physics*, Vol. 75, 062501 (2012).

DOI: [10.1088/0034-4885/75/6/062501](https://doi.org/10.1088/0034-4885/75/6/062501)

In this manuscript an understandable theoretical-experimental review of defects and doping in graphenic structures is presented.

8.- Terrones, H., Del Corro, E. Feng, S. , Poumirol, J.M., Rhodes, D., Smirnov, D., Pradhan, N.R., Lin, Z., Nguyen, M.A.T., Elías, A.L., Mallouk, T.E., Balicas, L., Pimenta, M.A., Terrones, M., ``New First Order Raman-active Modes in Few Layered Transition Metal Dichalcogenides", *Scientific Reports*, Vol. 4, 4215 (2014).

DOI: [10.1038/srep04215](https://doi.org/10.1038/srep04215)

In this manuscript new Raman modes are calculated theoretically and found experimentally for few layers of different transition metal dichalcogenides (MoS₂, WS₂, WSe₂, MoSe₂).