

Supplementary Information for:  
Oxidation-dependent mechanical response of  
graphene oxide: taming the spread with ab-initio  
Machine Learning simulations

Sara Shahbazi Fashtali<sup>1\*</sup>, Pablo M. Piaggi<sup>2,3</sup> and Giuseppe Zollo<sup>1</sup>

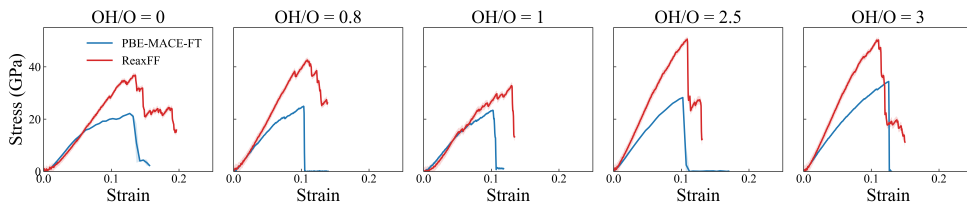
<sup>1\*</sup>Dipartimento di Scienze di Base e Applicate per l'Ingegneria,  
Sapienza University of Rome, A. Scarpa 14-16, Rome, 00161, Italy.

<sup>2</sup>CIC nanoGUNE, Tolosa Hiribidea 76, Donostia-San Sebastián, 20018,  
Spain.

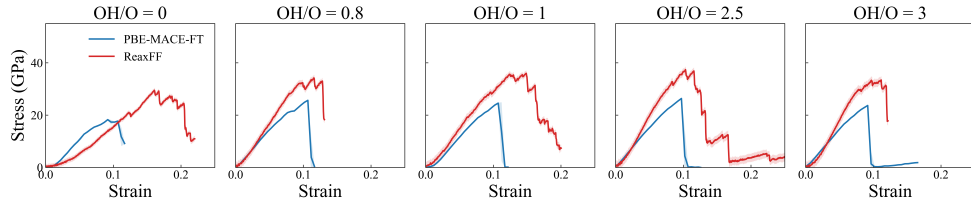
<sup>3</sup>Ikerbasque, Basque Foundation for Science, Bilbao, 48013, Spain.

## 1 Additional stress–strain curves

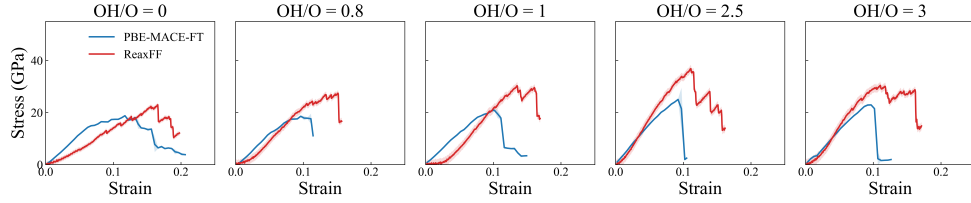
In this section, we report the full set of stress–strain curves for all investigated oxidation levels and hydroxyl-to-epoxy ratios. These results complement the representative curves shown in the main text and provide a complete overview of the mechanical response predicted by the PBE-MACE-FT and ReaxFF potentials.



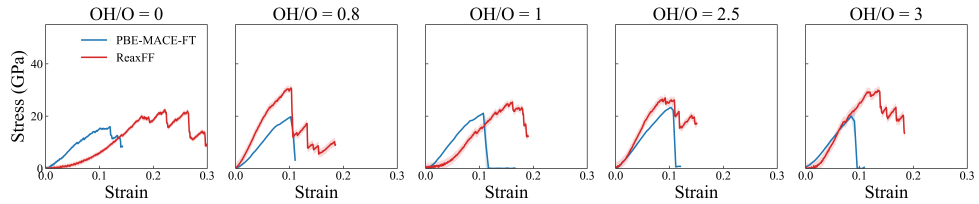
**Fig. 1** Stress–strain curves for graphene oxide with 10% oxidation at different OH/O ratios.



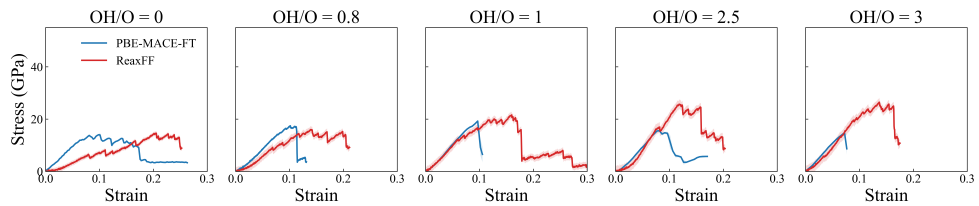
**Fig. 2** Stress-strain curves for graphene oxide with 20% oxidation at different OH/O ratios.



**Fig. 3** Stress-strain curves for graphene oxide with 25% oxidation at different OH/O ratios.

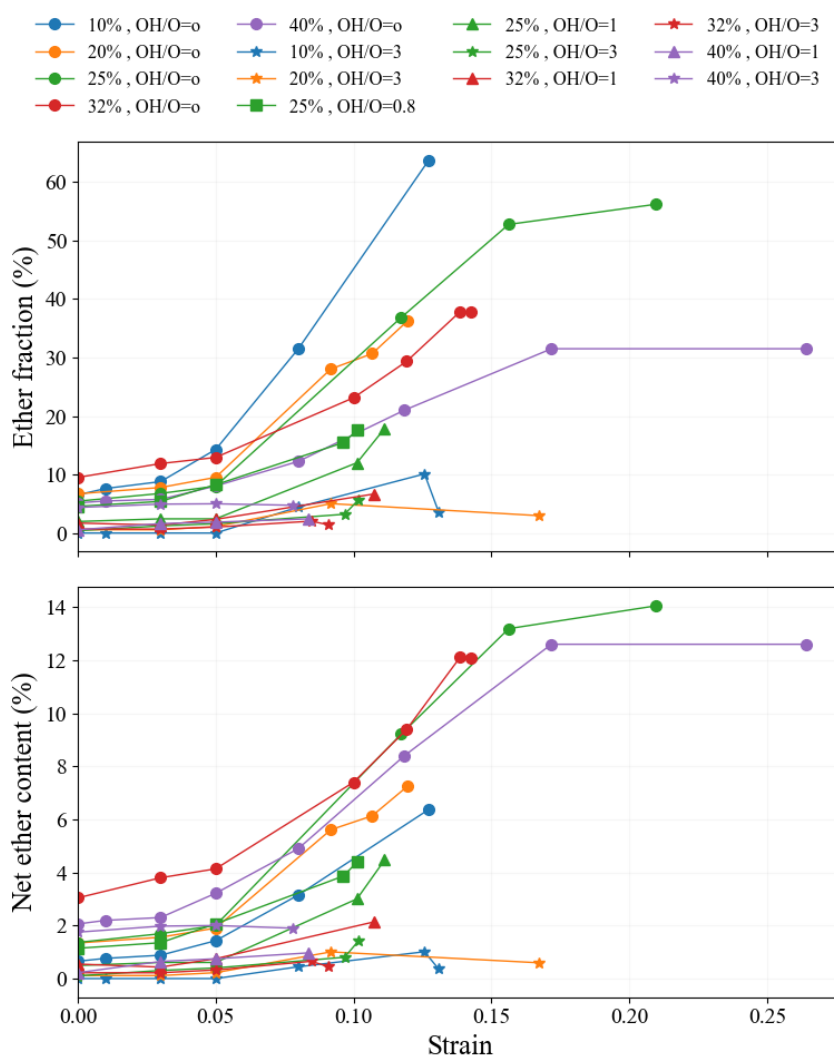


**Fig. 4** Stress-strain curves for graphene oxide with 32% oxidation at different OH/O ratios.



**Fig. 5** Stress-strain curves for graphene oxide with 40% oxidation at different OH/O ratios.

## 2 Evolution of ether configurations during deformation



**Fig. 6** Evolution of ether configurations during uniaxial deformation for GO systems with different oxidation levels and OH/O ratios. Top: Ether fraction, defined as the ratio of ether groups to the total number of oxygen-containing functional groups (ether, epoxy, and hydroxyl). Bottom: Effective ether content, defined as the product of the ether fraction and the oxidation level, representing the population of ether groups relative to carbon atoms. Each curve corresponds to a different oxidation level and functional group composition.