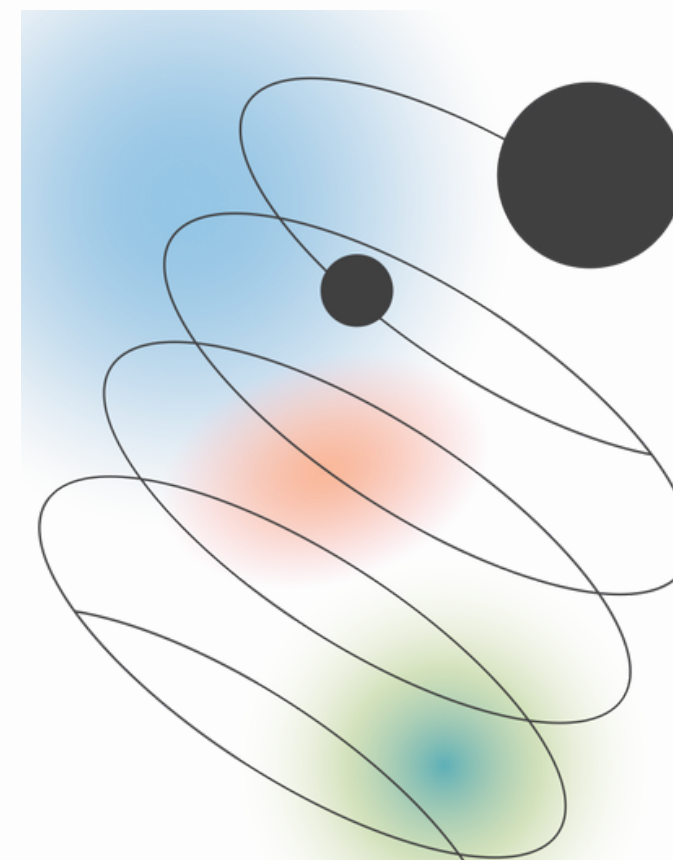
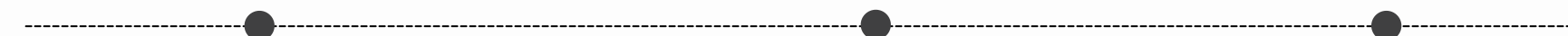


MD Simulation



THE JOURNAL OF
CHEMICAL PHYSICS

TETRAHEDRALITY OF BULK
WATER



A

AT 270K

B

AT 300 K

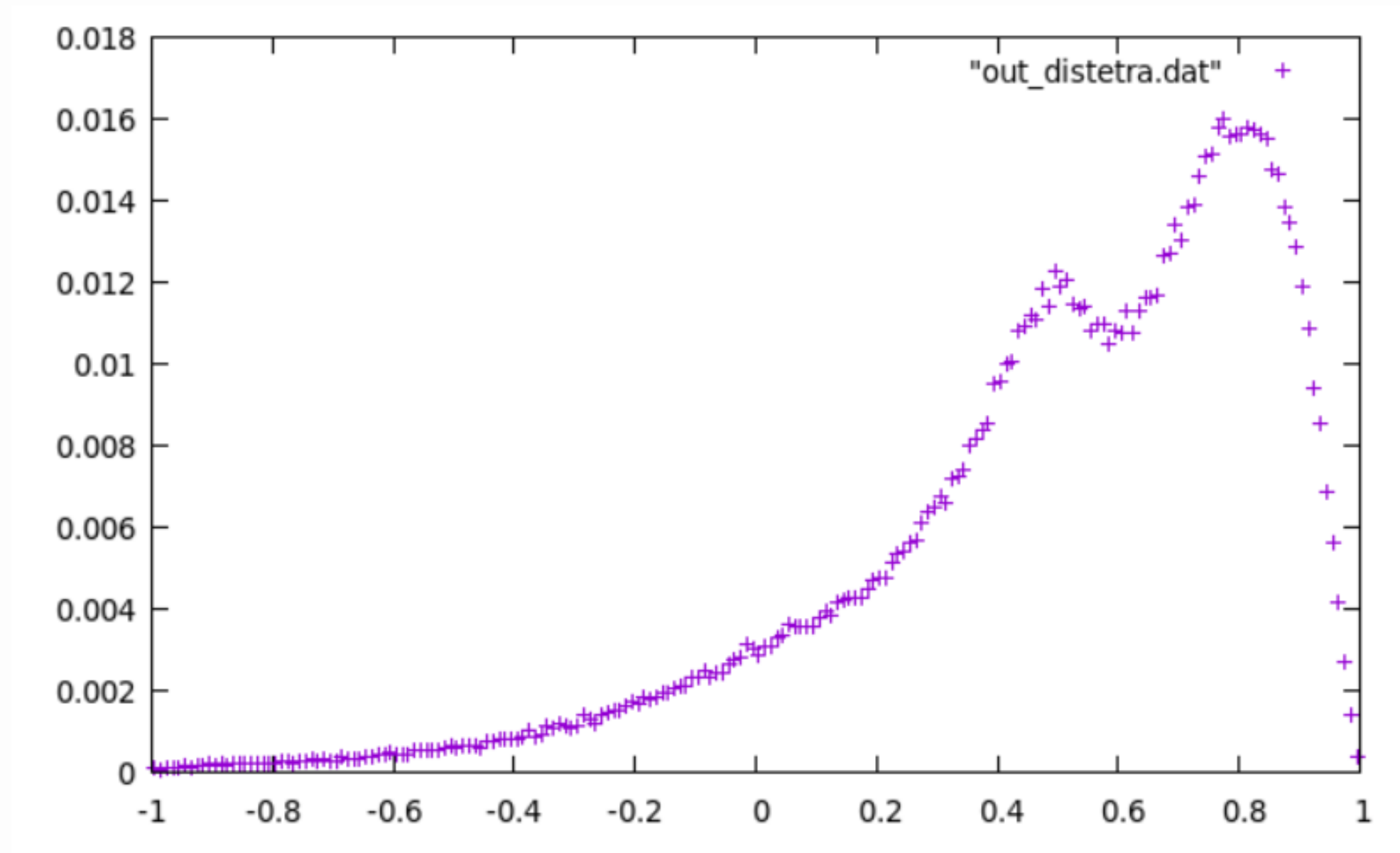
C

AT 330K

Effects of interfaces on structure and dynamics
of water droplets on a graphene surface: A
molecular dynamics study

A.

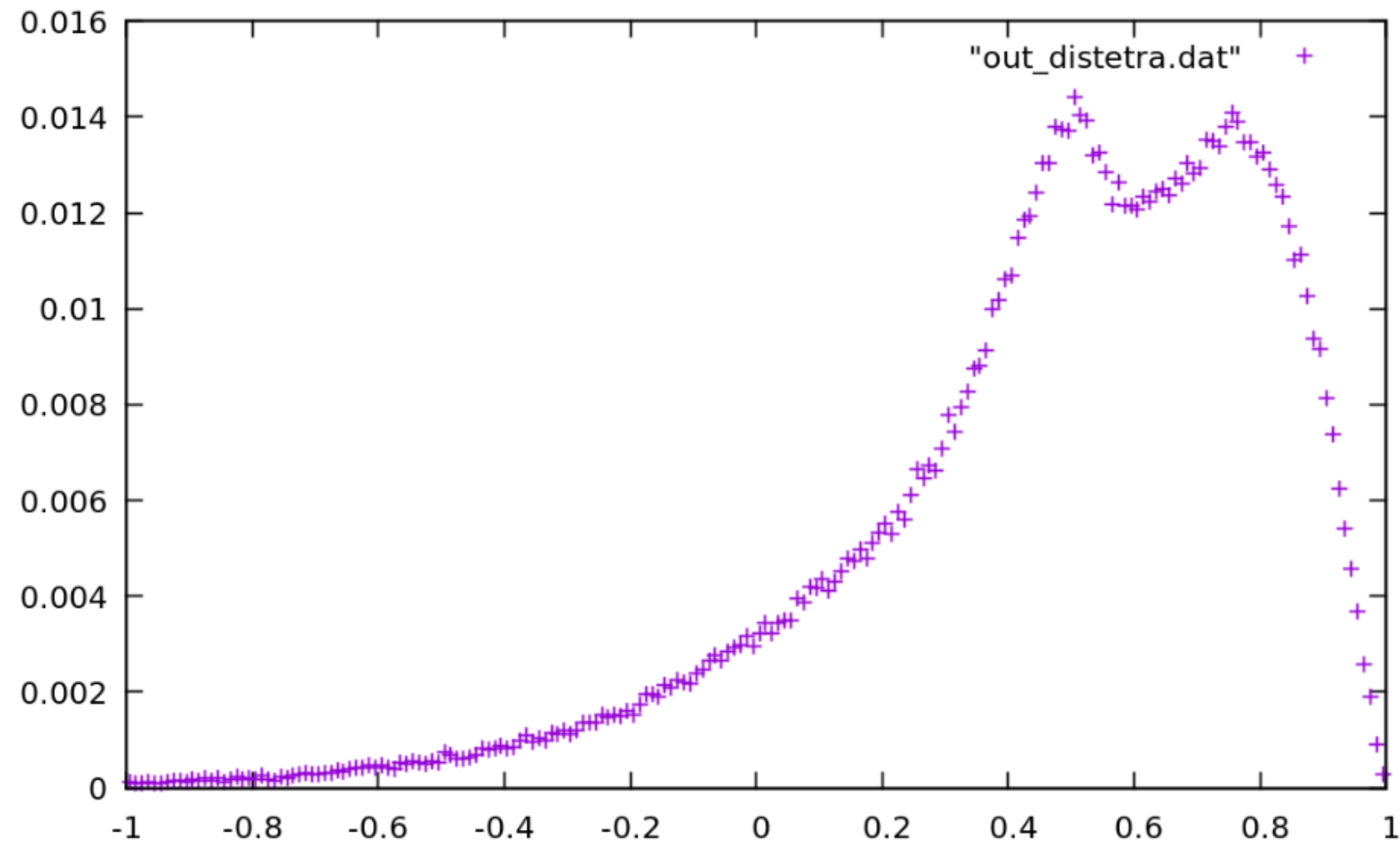
AT 270K



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B.

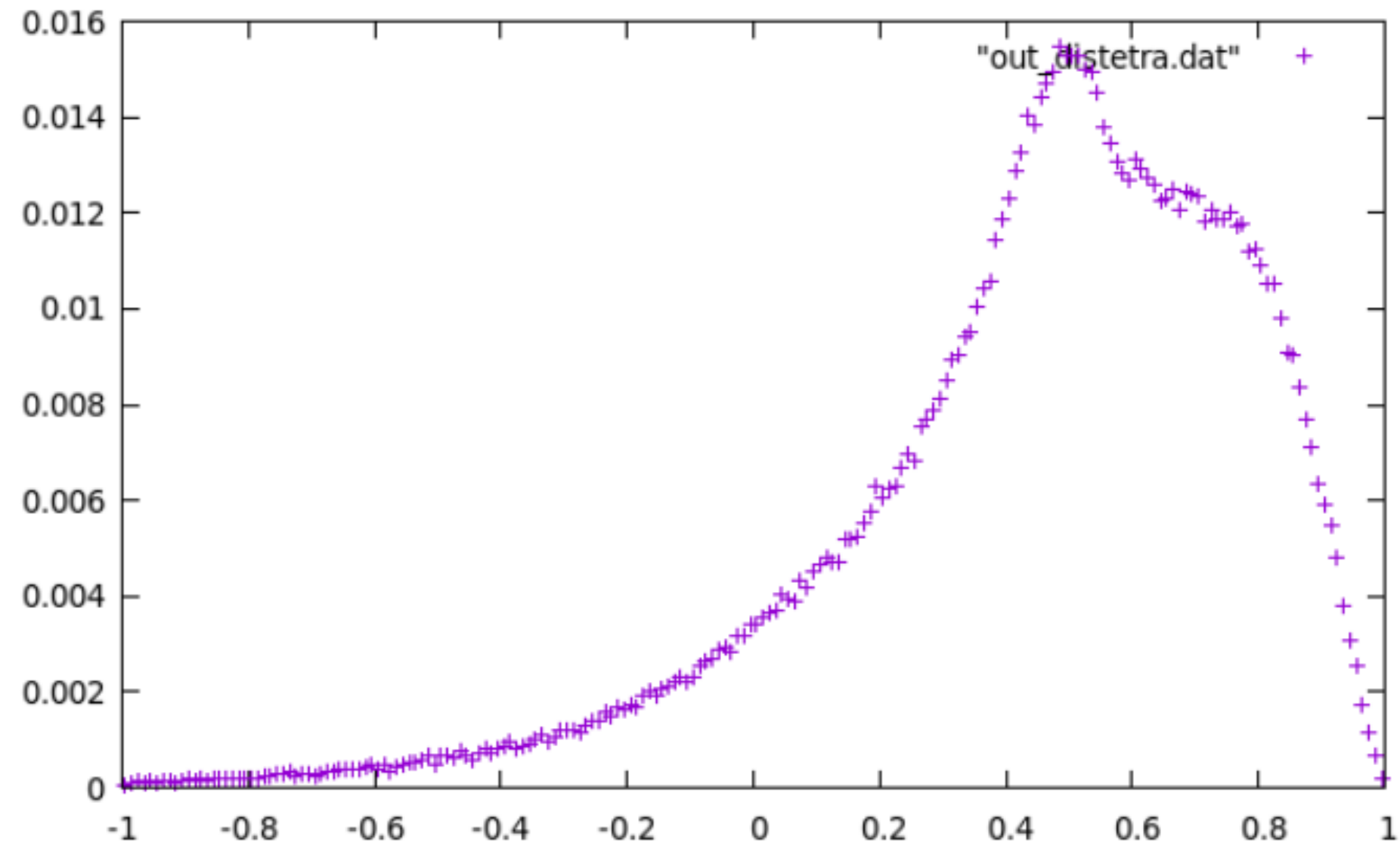
AT 300K



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300K\plot at 300K for tetrahedrality

C.

AT 330K



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D.

LITERATURE VALUE

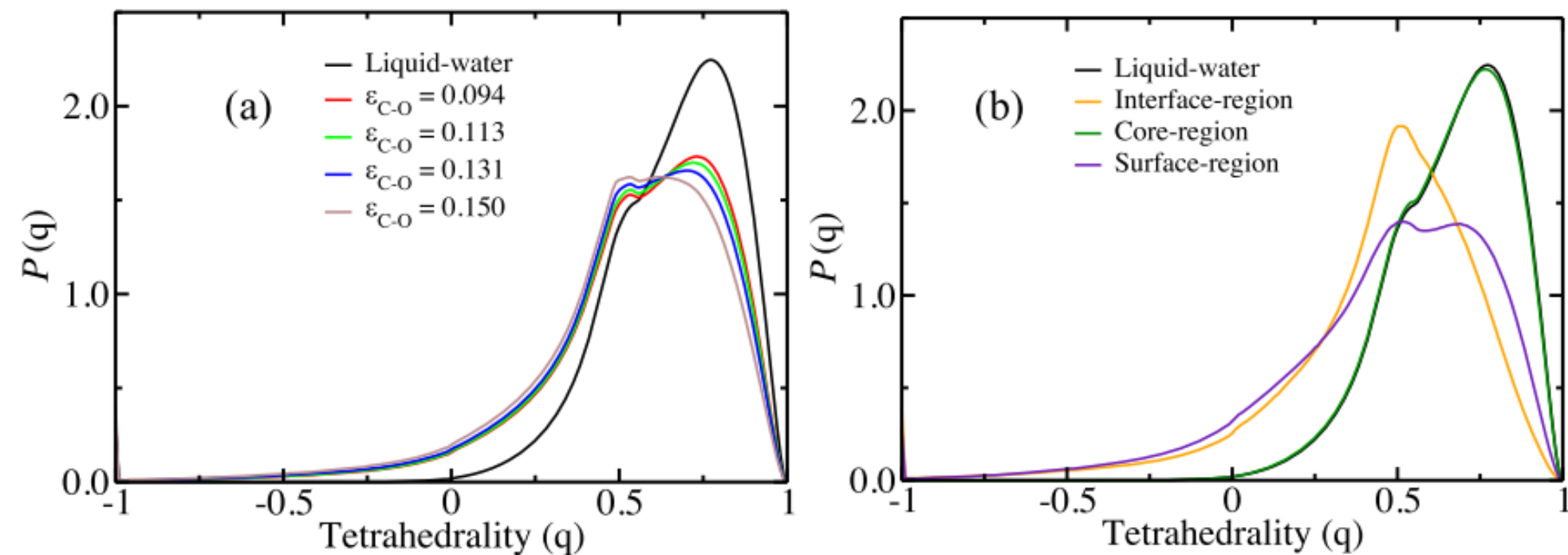


FIG. 6. (a) Probability distributions of the tetrahedral order parameter in a water droplet with different graphene–water interactions and liquid water. The color coding represents the increment in the LJ potential between the surface and water droplet, with red corresponding to the case of usual interaction with the surface. (b) Region-wise tetrahedral order parameter of water molecules in a water droplet with the usual interaction with the graphene surface. The tetrahedral order parameter of liquid water is also shown.

file:///C:/Users/asus/Desktop/Chem%202021%20project/Papers/2021_Effects%20of%20interfaces%20on%20structure%20and%20dynamics%20of%20water%20droplets%20on%20a%20graphene%20surface.pdf

THE END