Supplemental Information

Determination of Graphene Edges Energy using Hexagonal Graphene Quantum Dots and PM7 Method

Alexander V. Vorontsov[1,2]*, Evgeny V. Tretyakov[1,3]

[1] N. N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, pr. ak. Lavrentyeva 9, Novosibirsk 630090, Russia

[2] Altay State University, pr. Lenina 61, Barnaul 656049, Russia

3 Novosibirsk State University, Pirogova 2, Novosibirsk 630090, Russia

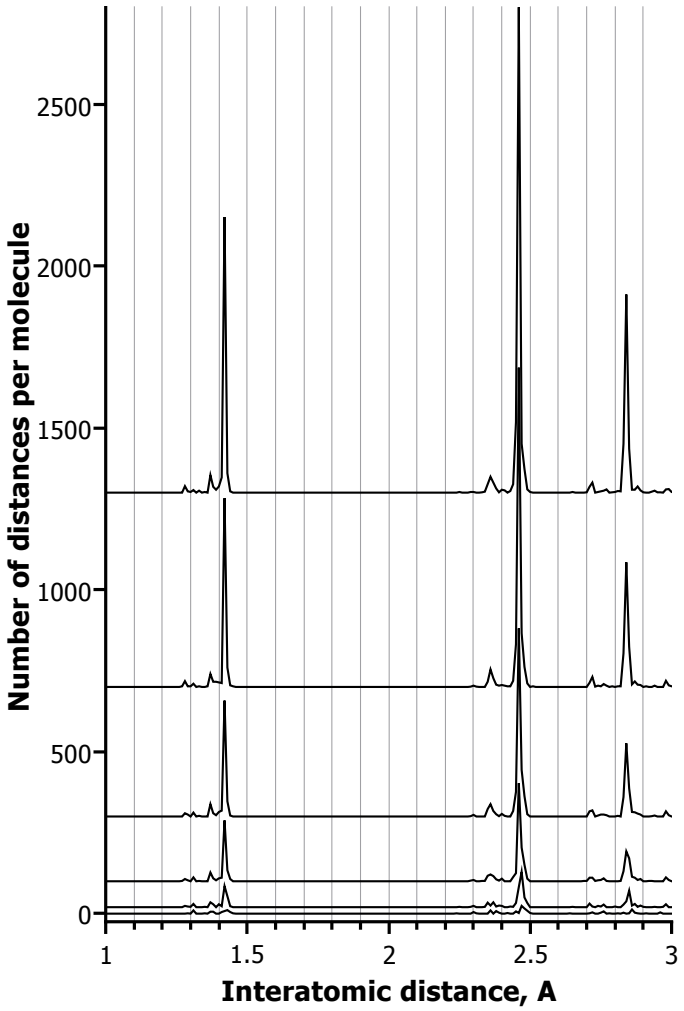

Fig. S1. Interatomic distance distribution function for GQD with armchair edge. From bottom to top: ac2, ac3, ac4, ac5, ac6, ac7.

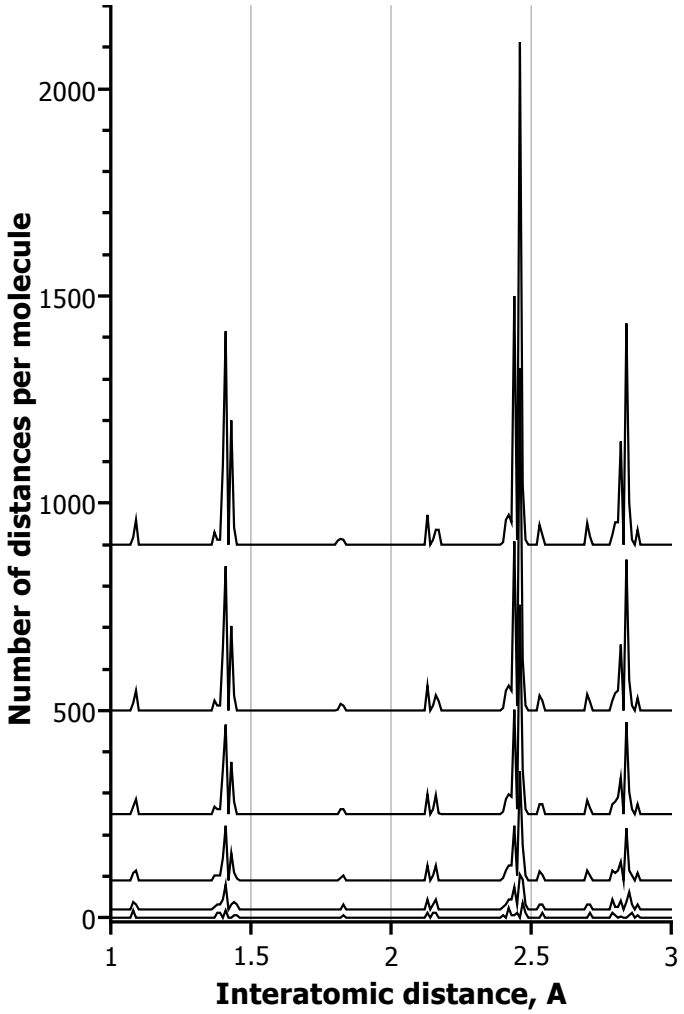

Fig. S2. Interatomic distance distribution function for hydrogen passivated armchair edge hexagonal graphene quantum dots. From bottom to top: ac2H to ac8H.

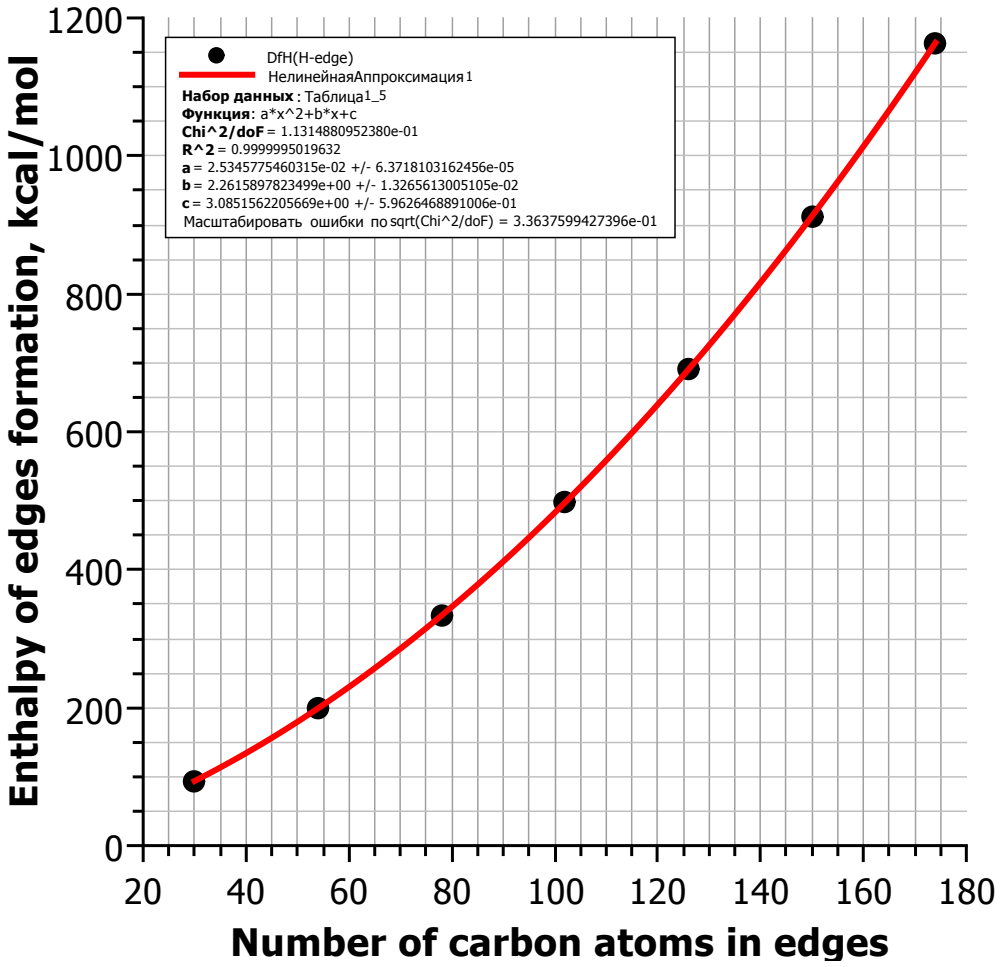

Fig. S3. Enthalpy of formation of hydrogenated edges of gqd-acXH graphene quantum dots as a function of number of carbon atoms in the edges.

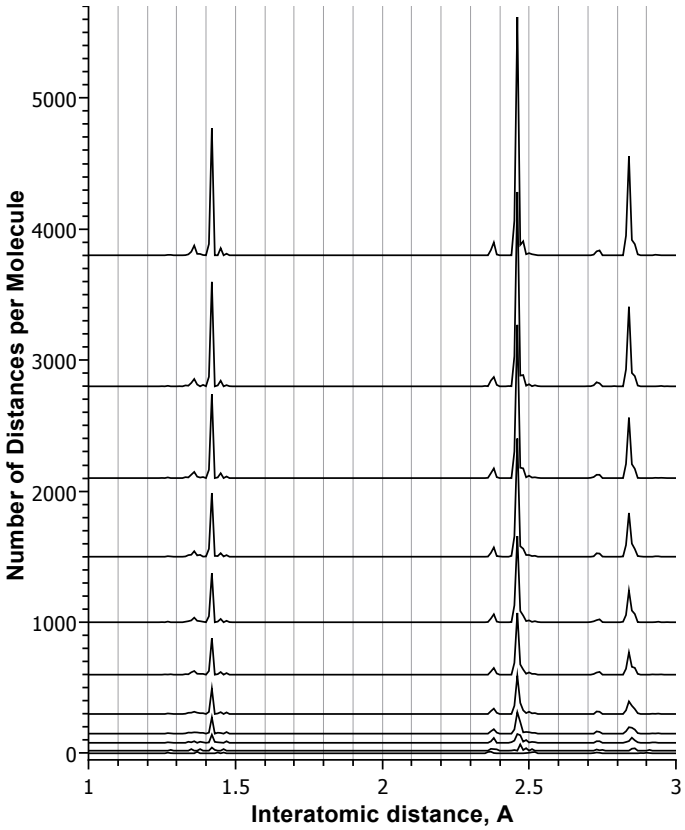

Fig. S4. Interatomic distance distribution function for graphene hexagonal quantum dots with zigzag edges. From bottom to top: zz2 to zz12.

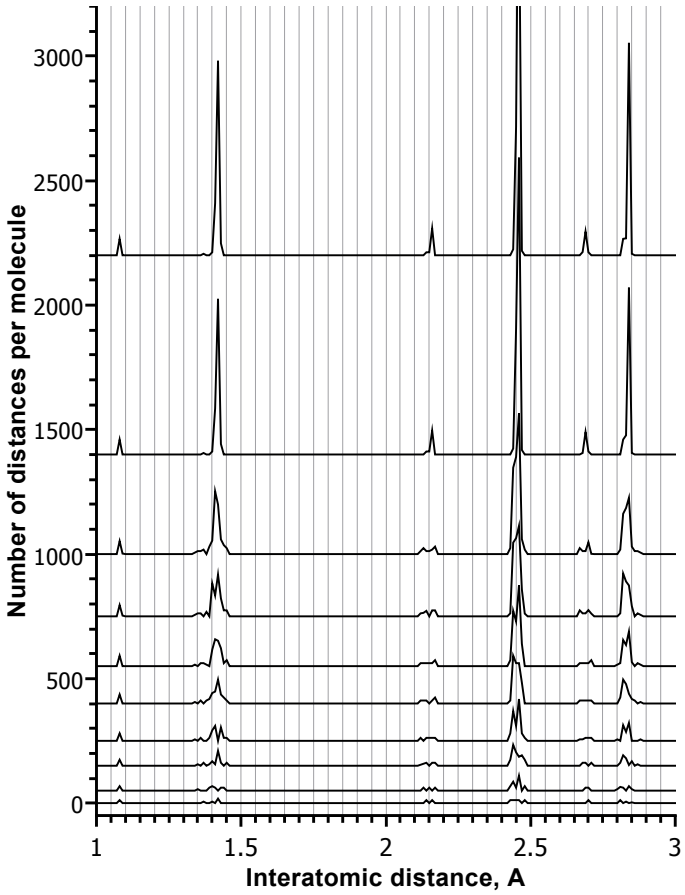

Fig. S5. Interatomic distance distribution function for hexagonal graphene quantum dots with hydrogen passivated zigzag edges. From bottom to top: zz2H to zz11H.

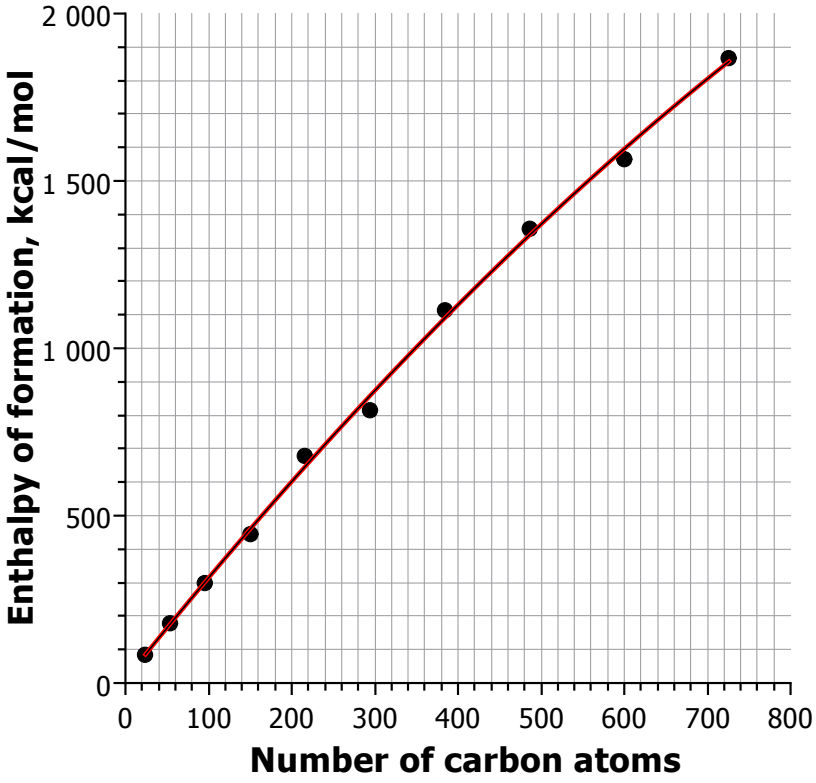

Fig. S6. Enthalpy of formation of graphene quantum dots with H-passivated zigzag edges plotted versus number of carbon atoms in GQDs. Computationally obtained points are approximated with quadratic function $y = (-0.000780 \pm 0.000189)\ x^2 + (3.11 \pm 0.14)\ x + (11.2 \pm 19.7)$.

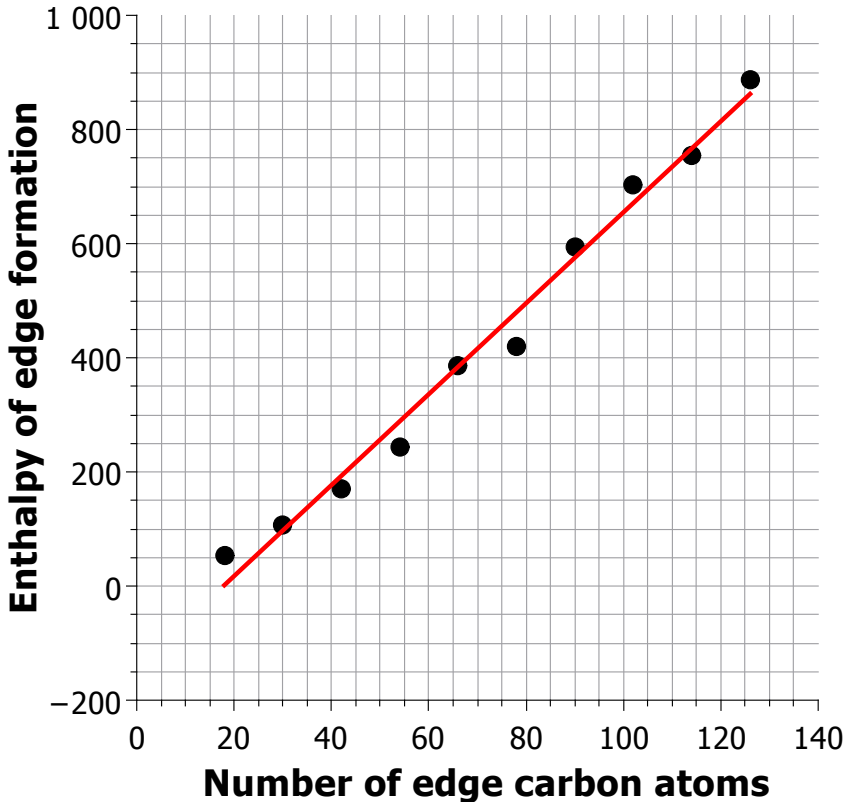

Fig. S7. Enthalpy of formation of hydrogenated zigzag edge of GQD as a function of number of edge carbon atoms. The points are fitted to linear function y = (7.97±0.34) x + (-142±27).