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The average values of tensor components of transport properties vs. chemical potential (μ) for pristine graphene and it derivatives (H_2S adsorbed on bridge, hollow and top-site configuration) at 300 and 600K are shown in Fig.1-4.

It is clear from Fig.1a,b that the p type carrier concentration shows greater average electrical conductivity (σ^{av}) as compared to n type carrier concentration for the two temperatures 300 K and 600 K. The σ^{av} shows a maximum value of $421\times10^{6}(\Omega.m)^{-1}$, $190\times10^{6}(\Omega.m)^{-1}$, $290\times10^{6}(\Omega.m)^{-1}$ and $122\times10^{6}(\Omega.m)^{-1}$ for pristine graphene, bridge, top and hollow-site configurations at 300 K. When the temperature is increased to 600 K the σ^{av} reduces to $400\times10^{6}(\Omega.m)^{-1}$, $175\times10^{6}(\Omega.m)^{-1}$, $276\times10^{6}(\Omega.m)^{-1}$ and $104\times10^{6}(\Omega.m)^{-1}$ for pristine graphene, bridge, top and hollow-site configuration. This could be related to the fact that at high temperature the scattering of phonons with electrons increases resulting in decreases the electrical conductivity [1].

The highly oscillatory spectra of the Seebeck coefficient (S^{av}) for four cases (pristine graphene, bridge, hollow and top-site configurations) shows same contribution of electron and hole concentrations. Pristine graphene and hollow-site configuration shows a maximum value of about $210\mu V/K$ at 300 K and $126\mu V/K$ at 600 K. The bridge and top-site configuration shows a maximum value of $150\mu V/K$ and $540\mu V/K$ for 300 K which reduced to $100\mu V/K$ and $280\mu V/K$ at 600 K as shown in Fig.2b.

The thermal conductivity (k^{av}) elucidates maximum value of n type concentration for pristine graphene and its derivative except the hollow-site configuration at 600 K which shows same electron-hole contribution. Here we also present k^{av} in p type region. The pristine graphene shows maximum value of $31\times10^{2}W/mK$ at 300 K. The H_2S adsorbed on bridge, top and hollow-site results decrease in k^{av} to $11.5\times10^{2}W/mK$, $19.5\times10^{2}W/mK$ and $8.0\times10^{2}W/mK$, respectively. For higher temperatures 600 K, the k^{av} shows significant increase in pristine graphene ($67.5\times10^{2}W/mK$). The bridge, top and hollow-site configuration enhances the k^{av} to $24\times10^{2}W/mK$, $35\times10^{2}W/mK$ and $13\times10^{2}W/mK$ at 600 K as shown Fig.3b. The greater value of thermal conductivity results lower values of figure of merit (ZT) provided that the lattice thermal conductivity is assumed to be similar.

The power factor $(P = \sigma S^2)$ is the important quantity for measuring transport properties of thermoelectric materials. The calculated average power factor P^{av} for pristine graphene and its derivative at different temperatures are shown in Fig. 4a,b. As one moves from 300 K to 600 K the P^{av} of pristine graphene increases from $14\times10^{-3}W/mK^2$ to $27\times10^{-3}W/mK^2$ while for the bridge-site configuration it reduces from $31\times10^{-3}W/mK^2$ $27\times10^{-3}W/mK^2$. For the top-site it shows a dramatic increase with the shift of $40.5\times10^{-3}W/mK^2$. The hollow-site increases from $14\times10^{-3}W/mK^2$ to $22\times10^{-3}W/mK^2$ as shown in Fig.4b.

[1] J. Hone, M. Whitney, C. Piskoti, and A. Zettl, Phys. Rev. B 59, R2514–R2516 (1999)

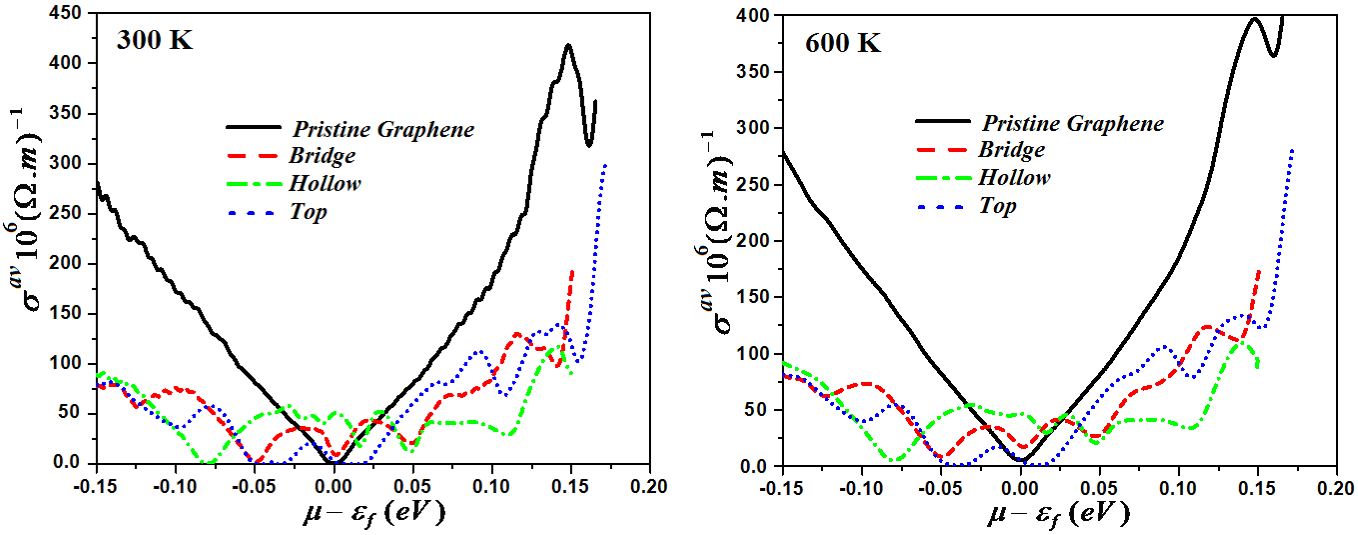
Figure Captions

Fig.1: Calculated average electrical conductivity (σ^{av}) of pristine graphene, H_2S adsorb on bridge site, H_2S adsorb on hollow site and H_2S adsorb on top site.

Fig.2: Calculated average Seebeck coefficient (S^{av}) of pristine graphene, H_2S adsorb on bridge site, H_2S adsorb on hollow site and H_2S adsorb on top site.

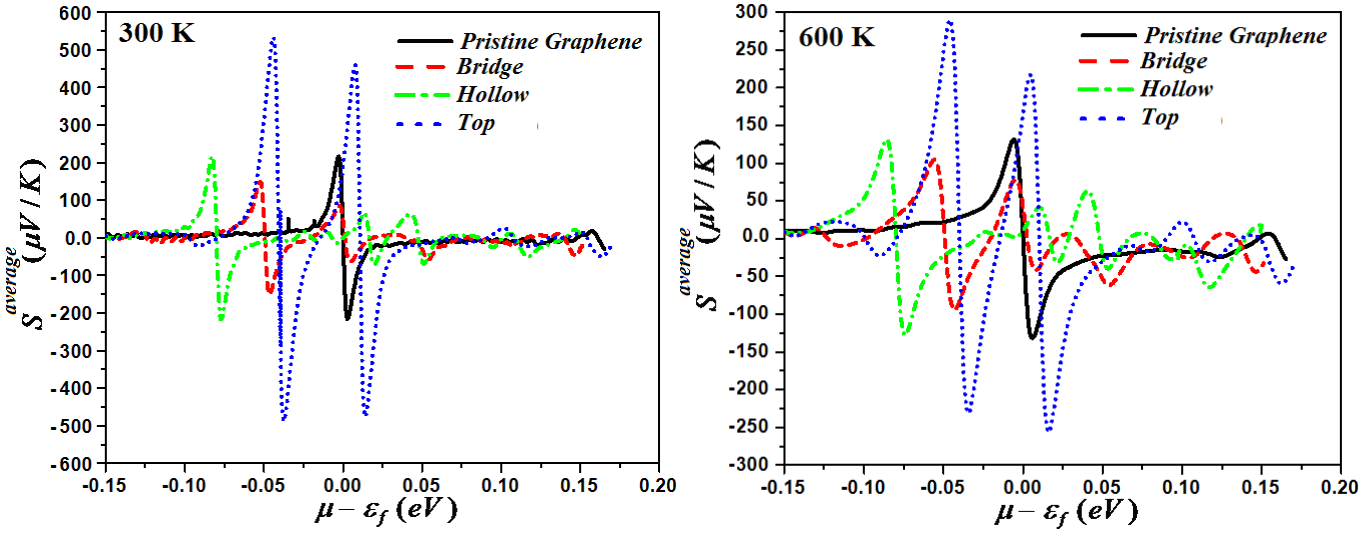
Fig.3: Calculated average thermal conductivity (k^{av}) of pristine graphene, H_2S adsorb on bridge site, H_2S adsorb on hollow site and H_2S adsorb on top site.

Fig.4: Calculated average value of power factor (P^{av}) of pristine graphene, H_2S adsorb on bridge site, H_2S adsorb on hollow site and H_2S adsorb on top site



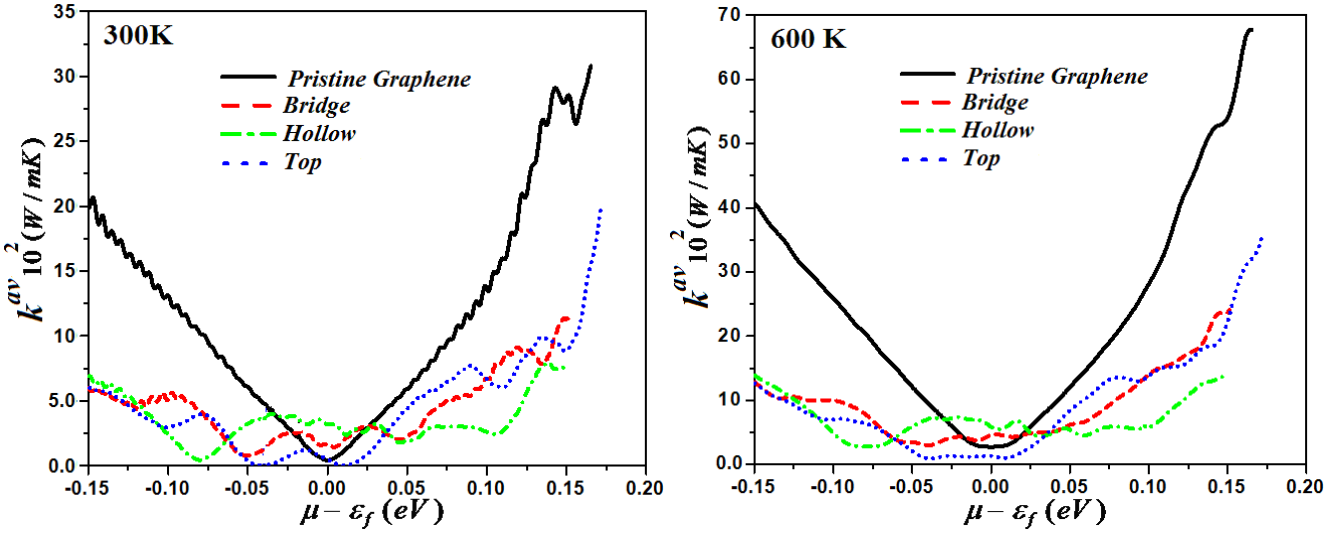
(a) (b)

Fig.1



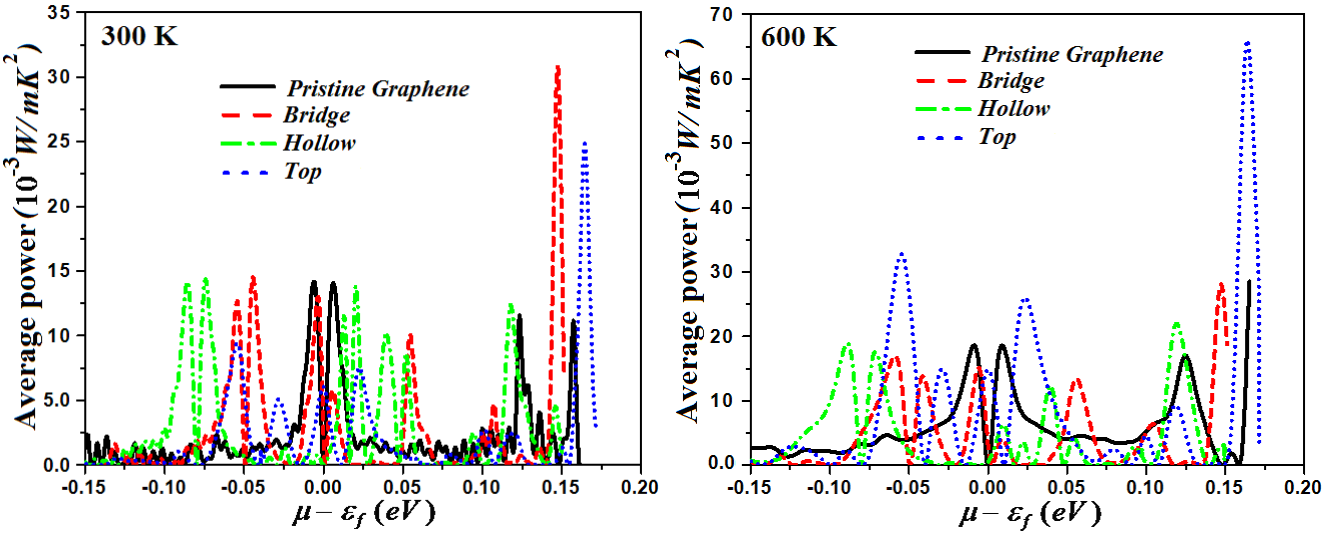
(a) (b)

Fig.2



(a) (b)

Fig.3



(g) (h)

Fig.4