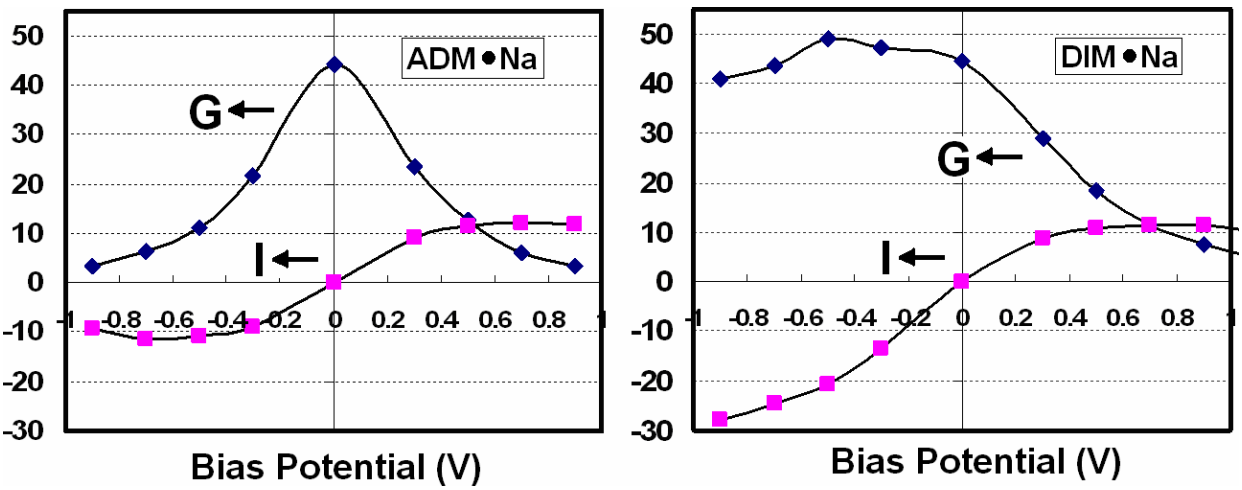

Fig. 4. **G**[μS] versus V[V] and I[μA] versus V[V] characteristics of ADM·Na and DIM·Na in linear electrodes corresponding to their horizontal orientations (Orientation 2 in Table 3).

molecules. Such information can be useful to build nanoscale active devices such as diodes or transistors. By studying the effects of applying various steady voltages or currents; we would find a desired mode of operation. As an example, we report horizontal orientation of these two molecules when placed in between Au linear electrodes as reported by Fig. 4. According to Fig. 4, there are plateaus in the I–V graph between 0.5 V and 0.9 V for both cases of ADM·Na and DIM·Na molecules and the currents come to maximums of 11.90 μA and 11.35 μA. Since the current is the integral of transmission over energy as in Eq. (1) and when bias V_b increases transmission $T(E, V_b)$ decreases, therefore the integral would come to a maximum, which is the reason for this plateau in the I–V characteristic graph. Using this I–V characteristic, we could build molecular rectifier or surge protector. Furthermore, two characteristics graph are obtained from the linear Au chain since only in the linear electrodes case we found peaks near Fermi energy, which show linear electrodes or atomic nanowire also have possibility to construct nanoscale devices for three-dimensional molecules.

5. Discussion

According to our first-principle studies of the three groups of diamondoids and derivatives, we could conclude that when different residues are added to diamondoids, the electronic properties of diamondoids can be changed, such as the HOMO–LUMO gap of molecules, the conductance, etc. We also found that the diamondoid derivatives have the potential as molecular building blocks of nanoscale electronic devices. The distance between the electrodes in the two cases depend on the orientation of the molecule in between the electrodes. Normally, in Au 2 × 2 electrodes case the conductance is greater than linear case, since when conductance is calculated, the central region is considered which includes some parts of the electrodes and there are more atoms in the 2×2 case. It is demonstrated that quantum conductance of diamondoid molecules and their derivative molecules change significantly by changing their orientations. The electronic property data and methodology generated are useful for building diamondoid-based NEMS and other nanoscale logic units.

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Appendix A. Abbreviations

ADM	Adamantane
ATK	Atomistix ToolKit
DFT	Density functional theory
DIM	Diamantane
DZP	Double zeta polarization
HOMO	Highest occupied molecular orbital
LDA-PZ	Perdew–Zunger local density approximation
LUMO	Lowest unoccupied molecular orbital
NEGF	Nonequilibrium Green's functions
Ry	Rydberg
VNL	Virtual Nanolab

Appendix B. Symbols

e	Electron charge
E	Energy
G	Conductance
G_0	Quantum conductance $2e^2/h = 77.5\,\mu$S
H	Hamiltonian
I	Current
T	Transmission
V_b	Bias potential
μS	10^{-6} Siemens

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