## Highlights

- The mechanism of surface charge-based sensing in asymmetrically functionalized nanopores is investigated using "Virtual EIS" tool and experiments .
- Virtual EIS tool can generate impedance spectrum from electric currents obtained by applying a step voltage input using a high-throughput code making it computationally efficient
- A way of enhancing sensitivity of the device is numerically explored and validated experimentally using thrombin and its aptamer system.