

## INTRODUCING MOLECULAR ELECTRONICS%0A

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4.3 Application of DFT to Modeling Molecular Electronics Devices . 120 4.4 Implementation: McDCAL,

TransSIESTA, and Atomistix Virtual NanoLab 134 4.5 Resistance of Molecular Wires 135 4.6.

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Molecular optoelectronics<sup>20, 21, 22</sup> is closely related to charge transport, but also involves electromagnetic interactions of higher frequency. It shares many mechanistic themes with charge transport. The third area is molecular magnetics, actuators, ferroelectrics and elastics<sup>23, 24</sup>.

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