In[•]:=
```
convertToAtomicUnit[q_Quantity] :=
  Module[{unitDimTable, atomicUnitTable, atomicUnit},
   unitDimTable = UnitDimensions[q];
   atomicUnitTable = unitDimTable /.
     {"ElectricCurrentUnit" → e Eh / ℏ , "LengthUnit" → a0 , "MassUnit" -> me ,
      "TimeUnit" -> ℏ / Eh , "AmountUnit" → mol / Avogadro numbers };
   atomicUnit = Times @@ Apply[Power[#1, #2] &, Transpose@atomicUnitTable];
   UnitConvert[q, atomicUnit]
  ];
convertToAtomicUnit[l_List] := convertToAtomicUnit /@ l;
convertFromAtomicUnit[q_Real, targetUnit_Quantity] :=
  Module[{unitDimTable, atomicUnitTable, atomicUnit},
   unitDimTable = UnitDimensions[targetUnit];
   atomicUnitTable = unitDimTable /.
     {"ElectricCurrentUnit" → e Eh / ℏ , "LengthUnit" → a0 , "MassUnit" -> me ,
      "TimeUnit" -> ℏ / Eh , "AmountUnit" → mol / Avogadro numbers };
   atomicUnit = Times @@ Apply[Power[#1, #2] &, Transpose@atomicUnitTable];
   UnitConvert[q * atomicUnit, targetUnit]
  ];
convertFromAtomicUnit[q_Real, targetUnit_String] :=
  convertFromAtomicUnit[q, Quantity[1, targetUnit] ];
convertFromAtomicUnit[q_Quantity, targetUnit_] := Module[{p},
   Assert[QuantityUnit[q], IndependentUnit["a.u."]];
   p = QuantityMagnitude[q];
   convertFromAtomicUnit[p, targetUnit]
  ];
convertFromAtomicUnit[l_List, targetUnit_] :=
  convertFromAtomicUnit[#, targetUnit] & /@ l;
```

In[•]:=
```
eq1 = pa + pb == 0;
```
$$eq2 = \frac{p_a^2}{2\, m_a} + \frac{p_b^2}{2\, m_b} == e_k;$$
```
sol = Solve[eq1~And~eq2, {pa, pb}] [[1]]
```

Out[•]= $$\left\{p_a \to -\frac{\sqrt{2}\,\sqrt{e_k}\,\sqrt{m_a}\,\sqrt{m_b}}{\sqrt{m_a+m_b}},\ p_b \to \frac{\sqrt{2}\,\sqrt{e_k}\,\sqrt{m_a}\,\sqrt{m_b}}{\sqrt{m_a+m_b}}\right\}$$

In[•]:=
```
data = {ek → 1.16 eV , ma -> sodium ELEMENT [ atomic mass ],
    mb -> chlorine ELEMENT [ atomic mass ]};
```

In[•]:=
```
moms = {pa, pb} /. sol /. data
```

Out[•]= $\{-5.68807\ \sqrt{u}\ \sqrt{eV},\ 5.68807\ \sqrt{u}\ \sqrt{eV}\}$

In[•]:=
```
convertToAtomicUnit[moms]
```

Out[•]= $\{-46.5554\ m_e\, a_0\, E_h/\hbar,\ 46.5554\ m_e\, a_0\, E_h/\hbar\}$

```
In[•]:= vels = {pa / ma, pb / mb} /. sol /. data
```

Out[•]= $\{-0.247418\ \sqrt{\text{eV}}/\sqrt{\text{u}},\ 0.160453\ \sqrt{\text{eV}}/\sqrt{\text{u}}\}$

```
In[•]:= convertToAtomicUnit[vels]
```

Out[•]= $\{-0.0011109\ a_0 E_h/\hbar,\ 0.000720433\ a_0 E_h/\hbar\}$

```
In[•]:= convertFromAtomicUnit[1.` a.u. , "eV"]
```

Out[•]= 27.2114 eV

```
In[•]:= convertFromAtomicUnit[1.` a.u. , s J ]
```

Out[•]= 1.05457×10^{-34} s J

```
In[•]:= convertFromAtomicUnit[1.` a.u. , "kcal/mol"]
```

Out[•]= 627.509 kcal_{th}/mol

```
In[•]:= convertFromAtomicUnit[1.` a.u. , "kj/mol"]
```

Out[•]= 2625.5 kJ/mol