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In[ ]:= convertToAtomicUnit[q_Quantity] :=
Module[{unitDimTable, atomicUnitTable, atomicUnit},
unitDimTable = UnitDimensions[q];
atomicUnitTable = unitDimTable /.
{"ElectricCurrentUnit" ->  $e E_h / \hbar$ , "LengthUnit" ->  $a_0$ , "MassUnit" ->  $m_e$ ,
"TimeUnit" ->  $\hbar / E_h$ , "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" ->  $e E_h / \hbar$ , "LengthUnit" ->  $a_0$ , "MassUnit" ->  $m_e$ ,
"TimeUnit" ->  $\hbar / E_h$ , "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 = p_a + p_b == 0;
eq2 =  $\frac{p_a^2}{2 m_a} + \frac{p_b^2}{2 m_b} == e_k$ ;
sol = Solve[eq1~And~eq2, {p_a, p_b}] [[1]]
Out[ ]:=  $\left\{ p_a \rightarrow -\frac{\sqrt{2} \sqrt{e_k} \sqrt{m_a} \sqrt{m_b}}{\sqrt{m_a + m_b}}, p_b \rightarrow \frac{\sqrt{2} \sqrt{e_k} \sqrt{m_a} \sqrt{m_b}}{\sqrt{m_a + m_b}} \right\}$ 

In[ ]:= data = {e_k -> 1.16 eV, m_a -> sodium ELEMENT [ atomic mass ],
m_b -> chlorine ELEMENT [ atomic mass ] };

In[ ]:= moms = {p_a, p_b} /. sol /. data
Out[ ]:=  $\{-5.68807 \sqrt{u} \sqrt{eV}, 5.68807 \sqrt{u} \sqrt{eV}\}$ 

In[ ]:= convertToAtomicUnit[moms]
Out[ ]:=  $\{-46.5554 m_e a_0 E_h / \hbar, 46.5554 m_e a_0 E_h / \hbar\}$ 

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In[*]:= vels = {pa / ma, pb / mb} /. sol /. data
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Out[*]:= { -0.247418  $\sqrt{\text{eV}} / \sqrt{u}$  , 0.160453  $\sqrt{\text{eV}} / \sqrt{u}$  }
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In[*]:= convertToAtomicUnit[vels]
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Out[*]:= { -0.0011109  $a_0 E_h / \hbar$  , 0.000720433  $a_0 E_h / \hbar$  }
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In[*]:= convertFromAtomicUnit[1.`a.u.` , "eV"]
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Out[*]:= 27.2114 eV
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In[*]:= convertFromAtomicUnit[1.`a.u.` , "s J"]
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Out[*]:=  $1.05457 \times 10^{-34}$  s J
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In[*]:= convertFromAtomicUnit[1.`a.u.` , "kcal/mol"]
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Out[*]:= 627.509 kcalth/mol
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In[*]:= convertFromAtomicUnit[1.`a.u.` , "kJ/mol"]
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Out[*]:= 2625.5 kJ/mol
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