Rovibrational Spectroscopy of Diatomic Molecules using Nikiforov-Uvarov Functional Analysis

Results

Symbols and Data

DO NOT run this cell (defining symbols) twice in the same notebook session. It will throw an error. If you want to evaluate the entire notebook, quit the kernel first.

In[•]:=
```
(*Define subscripted symbols*)
Notation`AutoLoadNotationPalette = False;
<< Notation`;
Symbolize /@ {De, re, X1, X2, X3, Enℓ, ψnℓ};
<< SciDraw`;
```

In[•]:=
```
(*Importing Dataset of Spectroscopic Constants*)
SetDirectory[NotebookDirectory[]];
molecularData =
 Import["data/molecular_data.csv", {"CSV", "Dataset"}, "HeaderLines" → {1, 1}]
```

Out[•]=

	D_e	r_e	mu	alpha
H2	4.7446	0.7416	0.50391	1.44056
LiH	2.51529	1.5956	0.880122	1.79984
HCl	4.61907	1.2746	0.980104	2.38057
CO	11.2256	1.1283	6.86067	2.59441
ScH	2.25	1.776	0.98604	2.50617
ScN	4.56	1.768	10.6828	2.66402
TiH	2.05	1.781	0.987371	2.35819
VH	2.33	1.719	0.988005	2.48172
CrH	2.13	1.694	0.988976	2.57791
NiC	2.76	1.621	9.97427	3.65206
CuLi	1.74	2.31	6.25949	2.3289
TiC	2.66	1.79	9.60608	2.73064
ScF	5.85	1.794	13.3589	2.62107
I2	1.5556	2.662	63.4522	4.96277
O2	5.15666	1.208	7.99746	0.999982

Parameters and Functions

In[•]:=
```
ħ = 1973.269804;
moleculesList =
  {"H2", "LiH", "HCl", "CO", "VH", "CrH", "CuLi", "TiC", "NiC", "ScN"};
(*function to get spectroscopic data for a chosen molecule*)
chooseMolecule[molecule_] :=
 ({De, re, μ, α} = {"D_e", "r_e", "mu", "alpha"} /. Normal[molecularData[molecule]];
  μ = μ * 9.3149410372 * 10^8; (*amu to eV/c^2*))

(*NUFA Definitions*)
β := 2 μ re^2 / (α^2 ħ^2);
X1 := De + ℓ (ℓ + 1) / (α^2 β) (3/α^2 - 1/α);
X2 := -2 De + ℓ (ℓ + 1) / (α^2 β) (-6/α^2 + 4/α);
X3 := ℓ (ℓ + 1) / (α^2 β) (1 + 3/α^2 - 3/α);
λ := Sqrt[β X1];
ν := Sqrt[β (-Enℓ + X3)];

(*Energy Equation*)
Enℓ := X3 - 1/β (1/2 + n + X2/2 Sqrt[β/X1])^2;

nonNormalizedEigenfunction[r_] :=
  FullSimplify[(e^(-λ z) z^ν Hypergeometric1F1[-n, (1 + 2 ν), 2 λ z]) /. {z → e^(-α (r - re)/re)}];
(*Normalization Constant*)
N := NIntegrate[(nonNormalizedEigenfunction[r])^2, {r, 0, ∞}];
(*Normalized Eigenfunction*)
ψnℓ[r_] := FullSimplify[1/Sqrt[N] nonNormalizedEigenfunction[r]];

(*Potential Functions*)
ModifiedMorse[r_] := De e^(-2 α (r - re)/re) - 2 De e^(-α (r - re)/re) + ħ^2/(2 μ) ℓ (ℓ + 1)/r^2;
pekerisApproximated[r_] := (X1 z^2 + X2 z + X3) /. {z → e^(-α (r - re)/re)};
```

Numerical Results and Test Plots

Eigenvalues

Basic Example

In[•]:=
```
(*Calculating an Energy Eigenvalue*)
(*adjust NumberForm arguments to control precision*)
chooseMolecule["LiH"]
n = 7;
ℓ = 10;
StringForm[
 "Energy Eigenvalue for `` under the Modified-Morse Potential; n = ``, ℓ = ``: `` eV",
 molecule, n, ℓ, NumberForm[E_nℓ, {20, 8}]]
```

Out[•]=
```
Energy Eigenvalue for molecule under the
  Modified-Morse Potential; n = 7, ℓ = 10: -1.29580533 eV
```

Table of Negative Eigenvalues

In[•]:=
```
chooseMolecule["ScN"]
nList = {0, 1, 2, 3, 4, 5};
ℓList = {0, 1, 2, 5, 10};

energyTable = Table[NumberForm[-E_nℓ, {20, 7}], {n, nList}, {ℓ, ℓList}];
(*column headings*)
energyTable = Prepend[%, ℓList];
(*row headings*)
energyTable = MapThread[Prepend, {%, Prepend[nList, "n\\ℓ"]}];
(*format to look like booktabs*)
energyTable = Grid[%, Dividers → {False, {{True, True}, -1 → True}},
  Alignment → Left, Spacings → {1, 1}]

(*Table[NumberForm[-E_nℓ,{20,7}],{n,nList},{ℓ,ℓList}]//Flatten//TableForm*)
```

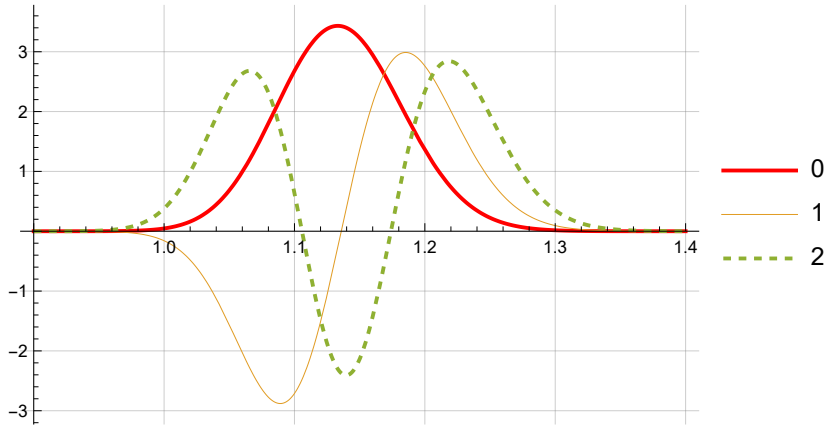
Out[•]=

n\ℓ	0	1	2	5	10
0	4.5151043	4.5149796	4.5147301	4.5132332	4.5082446
1	4.4259793	4.4258554	4.4256076	4.4241212	4.4191674
2	4.3377427	4.3376196	4.3373736	4.3358976	4.3309786
3	4.2503945	4.2502723	4.2500280	4.2485625	4.2436782
4	4.1639347	4.1638134	4.1635709	4.1621157	4.1572662
5	4.0783633	4.0782429	4.0780021	4.0765574	4.0717426

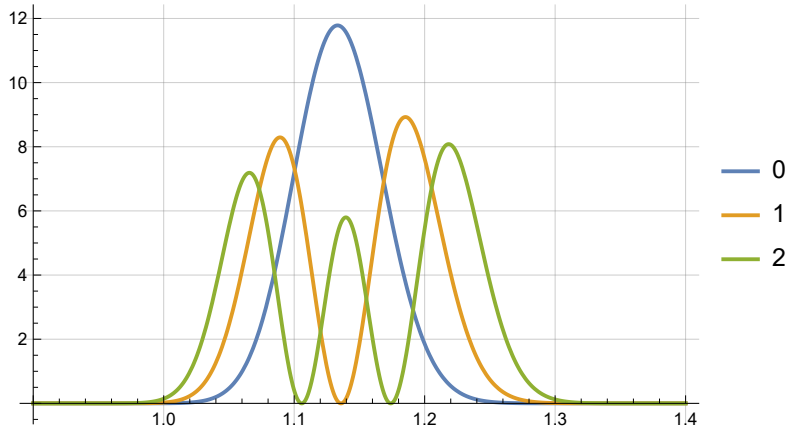
Eigenfunctions and Probability Densities

In[•]:=
```
chooseMolecule["CO"]
ℓ = 25;
Plot[Evaluate[Table[(ψ_nℓ[r]), {n, 0, 2}]],
 {r, 0.9, 1.4}, PlotRange → Full, PlotLegends → Range[0, 2],
 GridLines → Automatic, PlotStyle → {Red, Thickness[0.001], Dashed}]

Plot[Evaluate[Table[(ψ_nℓ[r])^2, {n, 0, 2}]], {r, 0.9, 1.4},
 PlotRange → Automatic, PlotLegends → Range[0, 2], GridLines → Automatic]
```

Out[•]=



Out[•]=



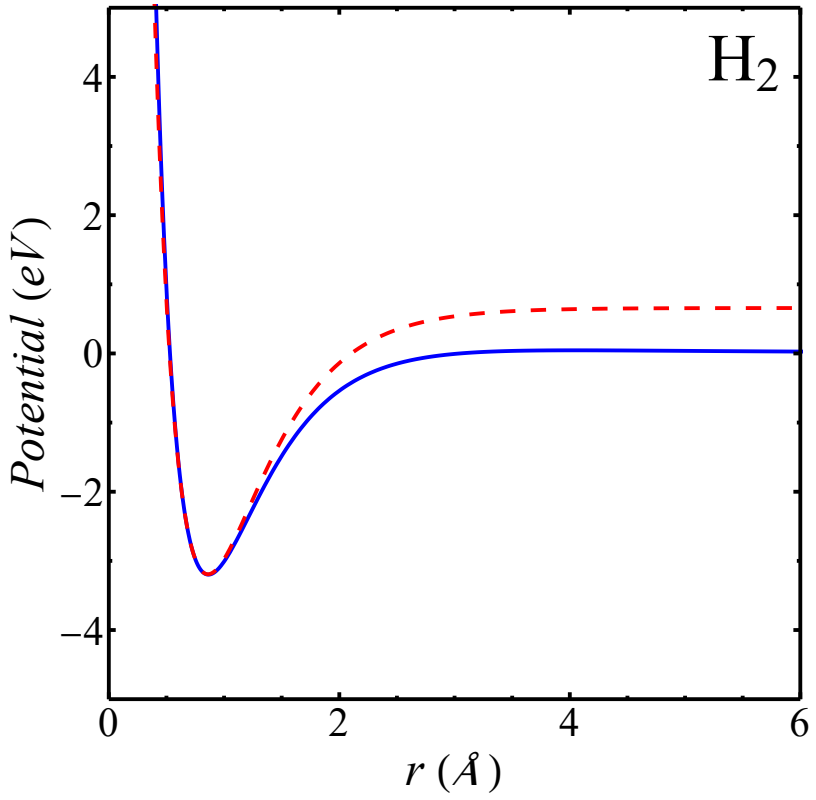
Plots for Publication

1. Potential Plots

H_2

In[•]:=
```
chooseMolecule["H2"]; ℓ = 15;
potentialPlotH2 = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.92, 0.92}], "H2", FontSize → 35];

    (*plots*)
    FigLine[
     Plot[ModifiedMorse[r], {r, 0.1, 10}, PlotRange → Full],
     LineColor → Blue, LineThickness → 2, LineDashing → 0
    ];
    FigLine[
     Plot[pekerisApproximated[r], {r, 0.1, 10}, PlotRange → Full],
     LineColor → Red, LineThickness → 2, LineDashing → 8
    ];
   },

   (*plot ranges*)
   XPlotRange → {0, 6}, XFrameLabel → textit["r (Å)"],
   YPlotRange → {-5, 5}, YFrameLabel → textit["Potential (eV)"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 6, 2, 4],
   YTicks → LinTicks[-4, 4, 2, 2],

   XTickLabelAllowance → 23,

   FontSize → 25,
   LineThickness → 2
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.8, 0.2}, {0.7, 0.2}}
 ]
```

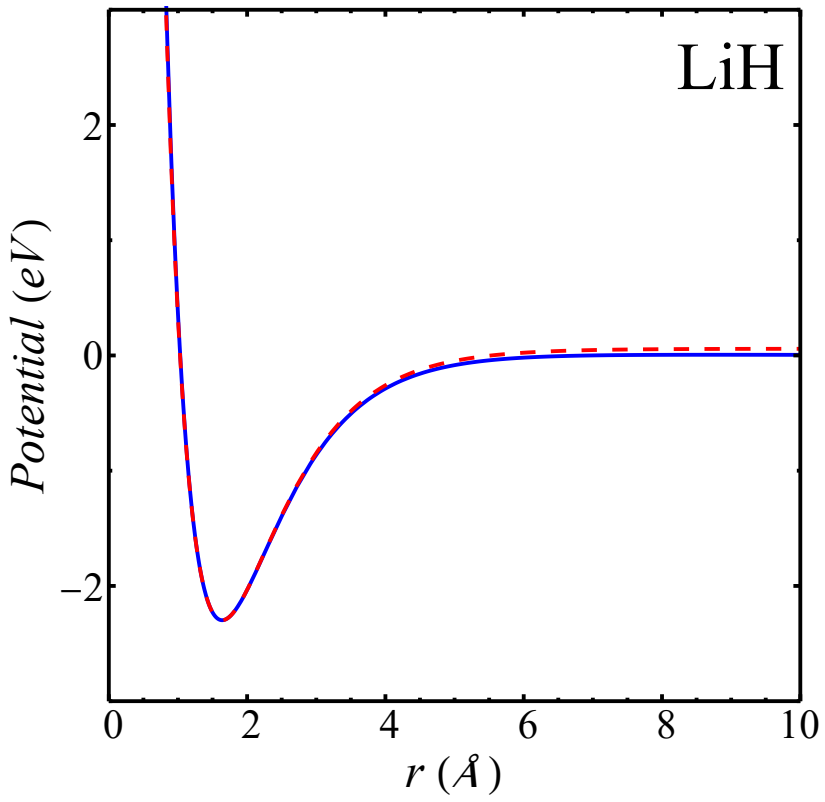
Out[•]=



LiH

In[•]:=
```
chooseMolecule["LiH"]; ℓ = 15;
potentialPlotLiH = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.9, 0.92}], "LiH", FontSize → 35];

    (*plots*)
    FigLine[
     Plot[ModifiedMorse[r], {r, 0.1, 10}, PlotRange → Full],
     LineColor → Blue, LineThickness → 2, LineDashing → 0
    ];
    FigLine[
     Plot[pekerisApproximated[r], {r, 0.1, 10}, PlotRange → Full],
     LineColor → Red, LineThickness → 2, LineDashing → 8
    ];
   },

   (*plot ranges*)
   XPlotRange → {0, 10}, XFrameLabel → textit["r (Å)"],
   YPlotRange → {-3, 3}, YFrameLabel → textit["Potential (eV)"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 10, 2, 4],
   YTicks → LinTicks[-4, 4, 2, 2],

   XTickLabelAllowance → 23,

   FontSize → 25,
   LineThickness → 2
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.8, 0.2}, {0.7, 0.2}}
 ]
```

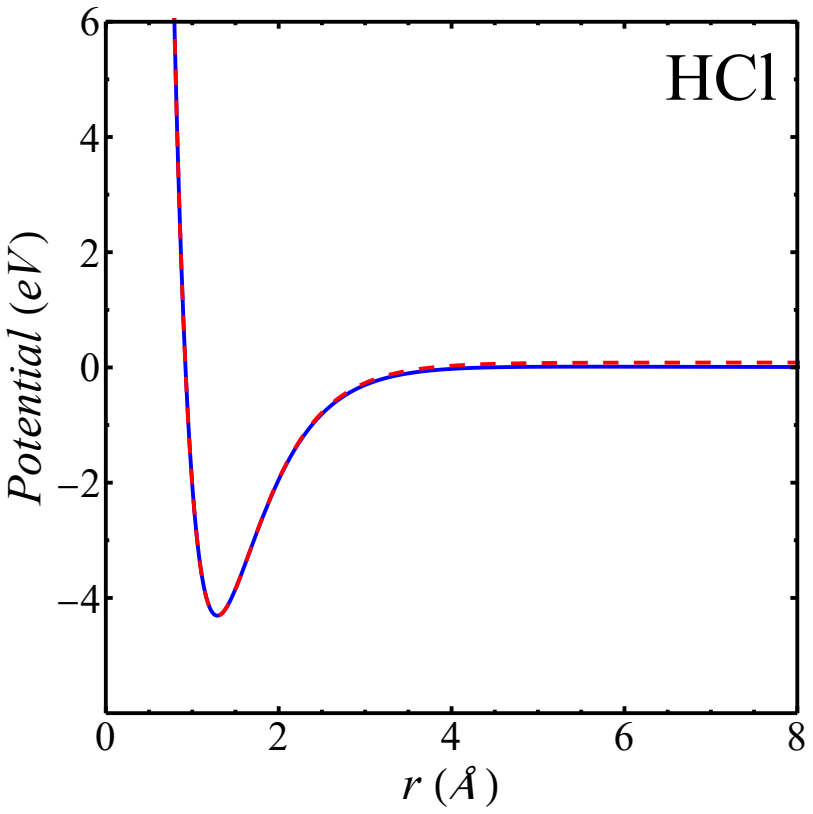
Out[•]=



HCl

In[ ]:=
```
chooseMolecule["HCl"]; ℓ = 15;
potentialPlotHCl = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.89, 0.92}], "HCl", FontSize → 35];

    (*plots*)
    FigLine[
     Plot[ModifiedMorse[r], {r, 0.1, 10}, PlotRange → Full],
     LineColor → Blue, LineThickness → 2, LineDashing → 0
    ];
    FigLine[
     Plot[pekerisApproximated[r], {r, 0.1, 10}, PlotRange → Full],
     LineColor → Red, LineThickness → 2, LineDashing → 8
    ];
   },

   (*plot ranges*)
   XPlotRange → {0, 8}, XFrameLabel → textit["r (Å)"],
   YPlotRange → {-6, 6}, YFrameLabel → textit["Potential (eV)"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 8, 2, 4],
   YTicks → LinTicks[-4, 6, 2, 2],

   XTickLabelAllowance → 23,

   FontSize → 25,
   LineThickness → 2
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.8, 0.2}, {0.7, 0.2}}
 ]
```

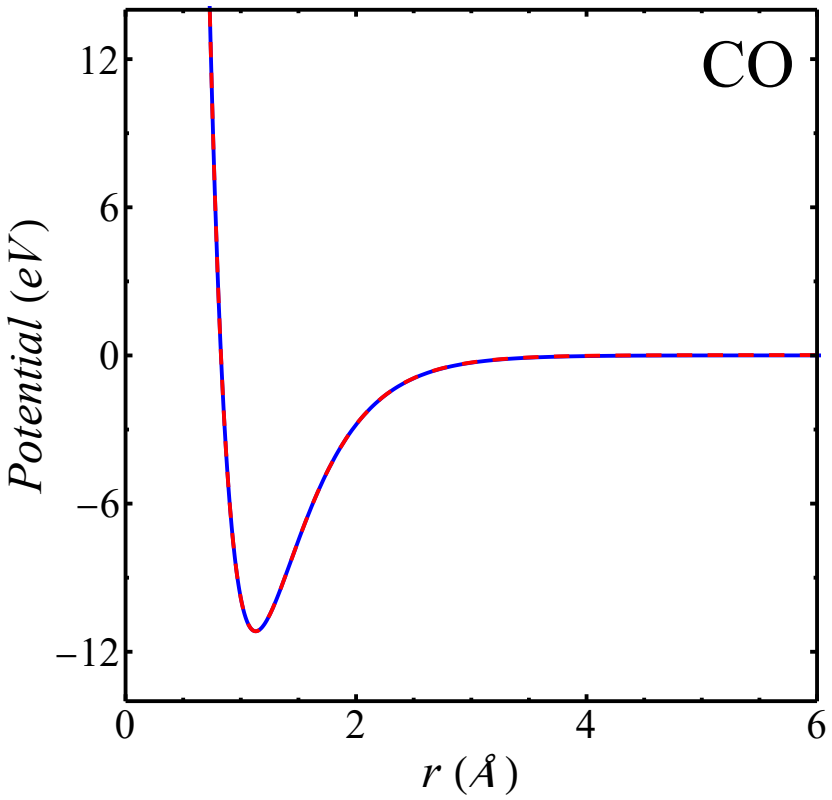
Out[•]=



CO

In[ ]:=
```
chooseMolecule["CO"]; ℓ = 15;
potentialPlotCO = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.9, 0.92}], "CO", FontSize → 35];

    (*plots*)
    FigLine[
     Plot[ModifiedMorse[r], {r, 0.1, 10}, PlotRange → Full],
     LineColor → Blue, LineThickness → 2, LineDashing → 0
    ];
    FigLine[
     Plot[pekerisApproximated[r], {r, 0.1, 10}, PlotRange → Full],
     LineColor → Red, LineThickness → 2, LineDashing → 8
    ];
   },

   (*plot ranges*)
   XPlotRange → {0, 6}, XFrameLabel → textit["r (Å)"],
   YPlotRange → {-14, 14}, YFrameLabel → textit["Potential (eV)"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 6, 2, 4],
   YTicks → LinTicks[-12, 12, 6, 2],

   XTickLabelAllowance → 23,

   FontSize → 25,
   LineThickness → 2
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.95, 0.2}, {0.7, 0.2}}
 ]
```

Out[•]=

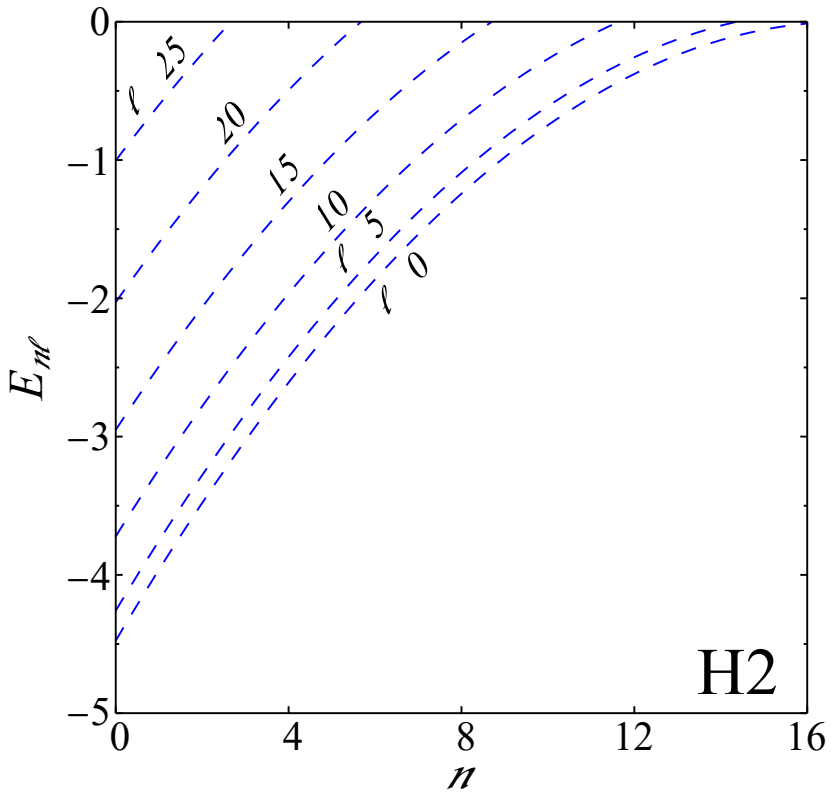


2. E_{nl} vs n

H_2

In[•]:=
```
chooseMolecule["H2"];
EnPlotH2 = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.9, 0.06}], "H2", FontSize → 35];

    (*plots*)
    Do[
     FigLine[
      (*match x-
       y plot ranges here with down below. Needed for correct label positioning.*)
      Plot[Eₙℓ, {n, 0, 16}, PlotRange → {Full, {-5, 0}}],
      (*the label of the lowest (ℓ=0) line is to the right, to reduce clutter.*)
      If[ℓ ≠ 0, LeftLabel → textit[StringForm["ℓ=``", ℓ]],
       RightLabel → textit[StringForm["ℓ=``", ℓ]]],
      (*positions adjusted so
       attached labels are roughly in the middle of the curves*)
      LeftLabelPosition → 0.5, RightLabelPosition → 0.48,
      FontSize → 20, LineColor → Blue, LineThickness → 1, LineDashing → 8
     ],
     {ℓ, 0, 25, 5}]
   },

   (*plot ranges*)
   XPlotRange → {0, 16}, XFrameLabel → textit["n"],
   YPlotRange → {-5, 0}, YFrameLabel → textit["Eₙℓ"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 16, 4, 1],
   YTicks → LinTicks[-5, 0, 1, 2],
   (*to make space between ticks and axis labels*)
   XTickLabelAllowance → 24,
   YTickLabelAllowance → 29,

   FontSize → 25,
   LineThickness → 1
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
 ]
```

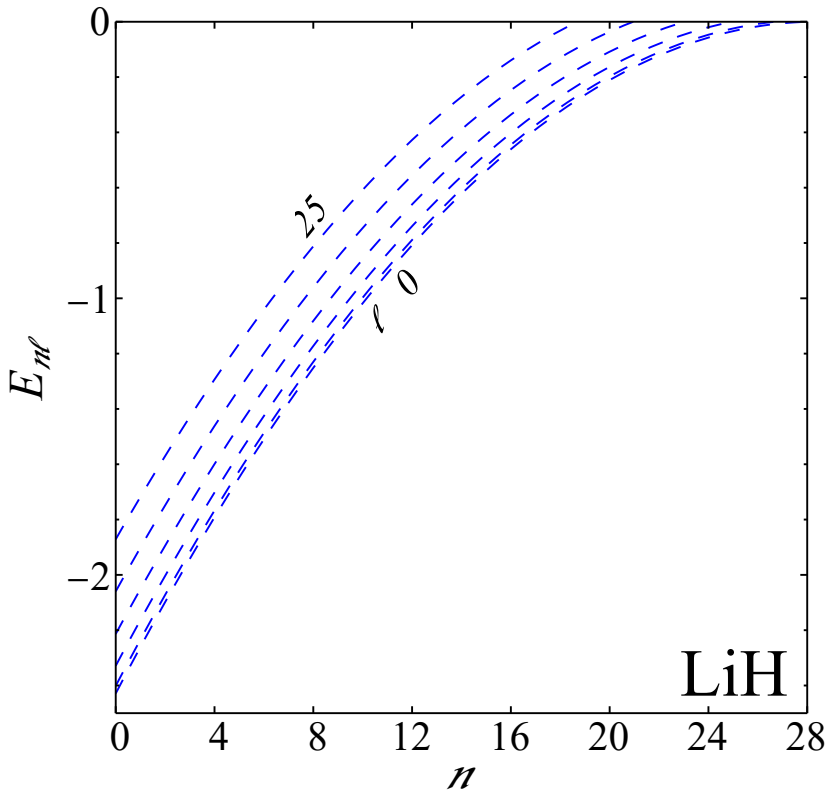
Out[•]=



LiH

In[•]:=
```
chooseMolecule["LiH"];
EnPlotLiH = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.895, 0.06}], "LiH", FontSize → 35];

    (*plots*)
    Do[
     FigLine[
      (*match x-
       y plot ranges here with down below. Needed for correct label positioning.*)
      Plot[E_nℓ, {n, 0, 28}, PlotRange → {Full, {-2.5, 0}}],
      (*the label of the lowest (ℓ=0) line is to the right, to reduce clutter.*)
      Which[ℓ == 0, RightLabel → textit[StringForm["ℓ=``", ℓ]],
       ℓ == 25, LeftLabel → textit[StringForm["ℓ=``", ℓ]],
       MemberQ[{5, 10, 15, 20}, ℓ], LeftLabel → ""],
      (*positions adjusted so
       attached labels are roughly in the middle of the curves*)
      LeftLabelPosition → 0.5, RightLabelPosition → 0.48,
      FontSize → 20, LineColor → Blue, LineThickness → 1, LineDashing → 8
     ],
     {ℓ, 0, 25, 5}]
   },

   (*plot ranges*)
   XPlotRange → {0, 28}, XFrameLabel → textit["n"],
   YPlotRange → {-2.5, 0}, YFrameLabel → textit["E_nℓ"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 28, 4, 1],
   YTicks → LinTicks[-3, 0, 1, 5],
   (*to make space between ticks and axis labels*)
   XTickLabelAllowance → 24,
   YTickLabelAllowance → 29,

   FontSize → 25,
   LineThickness → 1
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
 ]
```

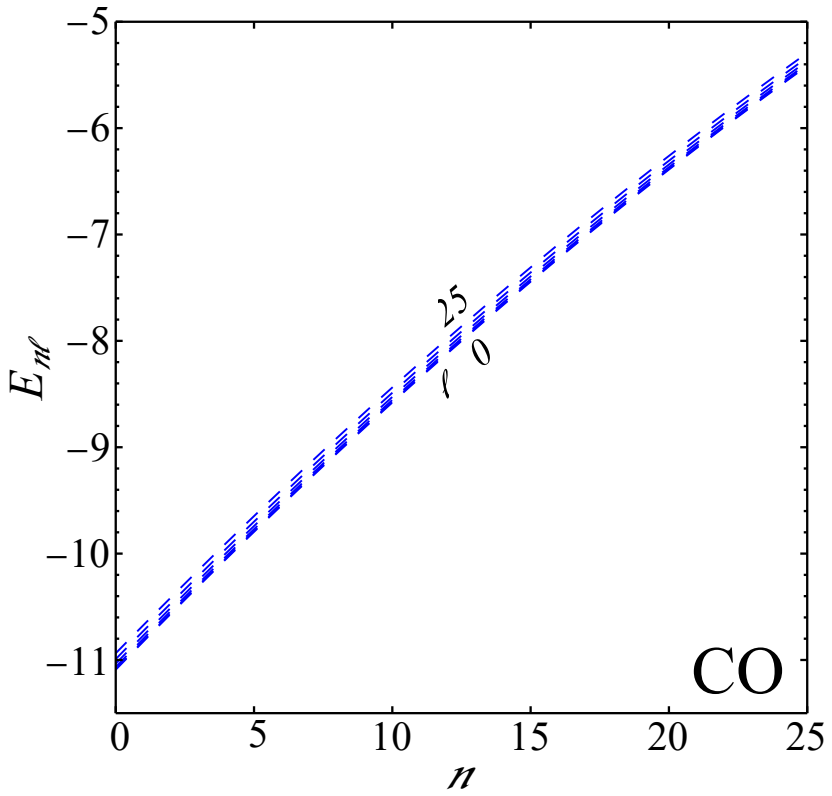
Out[•]=



CO

In[•]:=
```
chooseMolecule["CO"];
EnPlotCO = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.9, 0.06}], "CO", FontSize → 35];

    (*plots*)
    Do[
     FigLine[
      (*match x-
       y plot ranges here with down below. Needed for correct label positioning.*)
      Plot[E_nℓ, {n, 0, 25}, PlotRange → {Full, {-11.5, -5}}],
      (*the label of the lowest (ℓ=0) line is to the right, to reduce clutter.*)
      Which[ℓ == 0, RightLabel → textit[StringForm["ℓ=``", ℓ]],
       ℓ == 25, LeftLabel → textit[StringForm["ℓ=``", ℓ]],
       MemberQ[{5, 10, 15, 20}, ℓ], LeftLabel → ""],
      (*positions adjusted so
       attached labels are roughly in the middle of the curves*)
      LeftLabelPosition → 0.5, RightLabelPosition → 0.5,
      FontSize → 20, LineColor → Blue, LineThickness → 1, LineDashing → 8
     ],
     {ℓ, 0, 25, 5}]
   },

   (*plot ranges*)
   XPlotRange → {0, 25}, XFrameLabel → textit["n"],
   YPlotRange → {-11.5, -5}, YFrameLabel → textit["E_nℓ"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 25, 5, 1],
   YTicks → LinTicks[-11, 0, 1, 5],
   (*to make space between ticks and axis labels*)
   XTickLabelAllowance → 24,
   YTickLabelAllowance → 29,

   FontSize → 25,
   LineThickness → 1.2
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
 ]
```

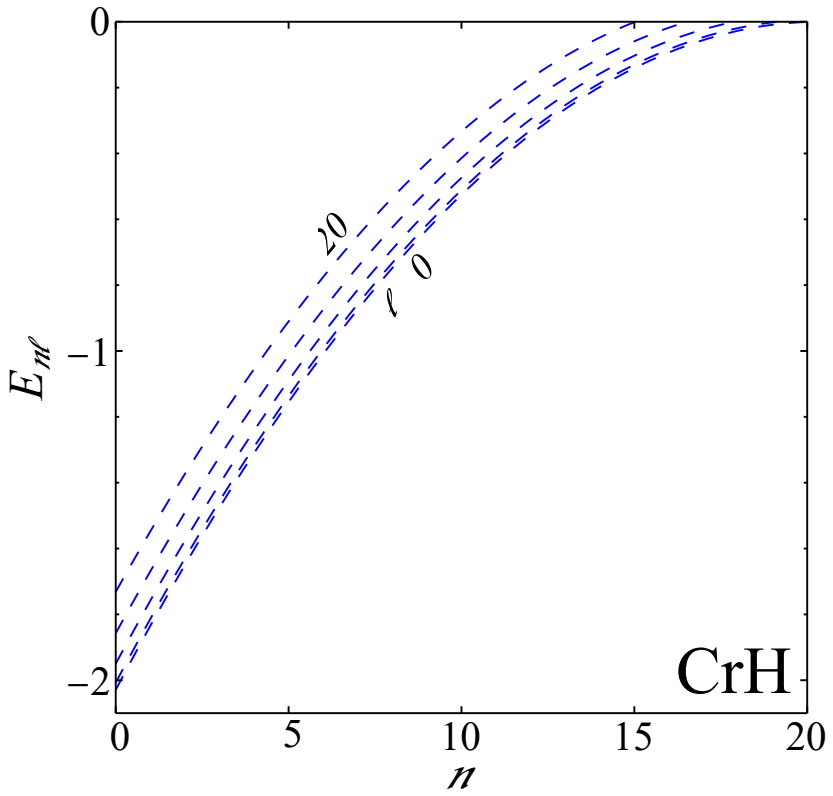
Out[•]=



CrH

In[•]:=
```
chooseMolecule["CrH"];
EnPlotCrH = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.895, 0.06}], "CrH", FontSize → 35];

    (*plots*)
    Do[
     FigLine[
      (*match x-
       y plot ranges here with down below. Needed for correct label positioning.*)
      Plot[E_nℓ, {n, 0, 20}, PlotRange → {Full, {-2.1, 0}}],
      (*the label of the lowest (ℓ=0) line is to the right, to reduce clutter.*)
      Which[ℓ == 0, RightLabel → textit[StringForm["ℓ=``", ℓ]],
       ℓ == 20, LeftLabel → textit[StringForm["ℓ=``", ℓ]],
       MemberQ[{5, 10, 15}, ℓ], LeftLabel → ""],
      (*positions adjusted so
       attached labels are roughly in the middle of the curves*)
      LeftLabelPosition → 0.5, RightLabelPosition → 0.5,
      FontSize → 20, LineColor → Blue, LineThickness → 1, LineDashing → 8
     ],
     {ℓ, 0, 20, 5}]
   },

   (*plot ranges*)
   XPlotRange → {0, 20}, XFrameLabel → textit["n"],
   YPlotRange → {-2.1, 0}, YFrameLabel → textit["E_nℓ"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 20, 5, 1],
   YTicks → LinTicks[-2, 0, 1, 5],
   (*to make space between ticks and axis labels*)
   XTickLabelAllowance → 24,
   YTickLabelAllowance → 29,

   FontSize → 25,
   LineThickness → 1
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
 ]
```

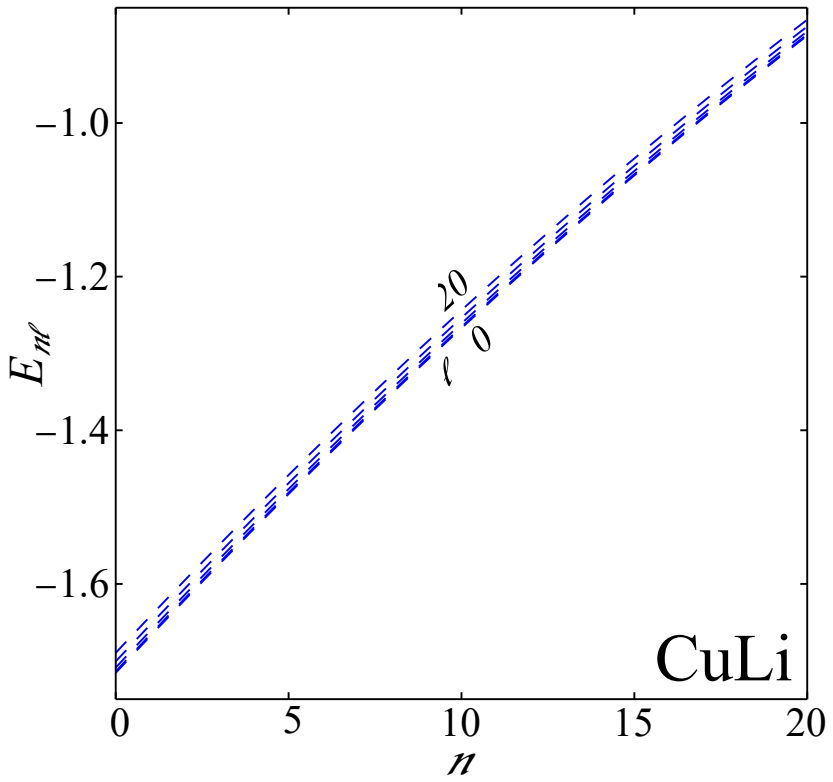
Out[•]=



CuLi

In[•]:=
```
chooseMolecule["CuLi"];
EnPlotCuLi = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.88, 0.06}], "CuLi", FontSize → 35];

    (*plots*)
    Do[
     FigLine[
      (*match x-
       y plot ranges here with down below. Needed for correct label positioning.*)
      Plot[E_n,ℓ, {n, 0, 20}, PlotRange → {Full, {-1.75, -0.85}}],
      (*the label of the lowest (ℓ=0) line is to the right, to reduce clutter.*)
      Which[ℓ == 0, RightLabel → textit[StringForm["ℓ=``", ℓ]],
       ℓ == 20, LeftLabel → textit[StringForm["ℓ=``", ℓ]],
       MemberQ[{5, 10, 15}, ℓ], LeftLabel → ""],
      (*positions adjusted so
       attached labels are roughly in the middle of the curves*)
      LeftLabelPosition → 0.5, RightLabelPosition → 0.5,
      FontSize → 20, LineColor → Blue, LineThickness → 1, LineDashing → 8
     ],
     {ℓ, 0, 20, 5}]
   },

   (*plot ranges*)
   XPlotRange → {0, 20}, XFrameLabel → textit["n"],
   YPlotRange → {-1.75, -0.85}, YFrameLabel → textit["E_n,ℓ"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 20, 5, 1],
   YTicks → LinTicks[-1.8, -0.8, 0.2, 1],
   (*to make space between ticks and axis labels*)
   XTickLabelAllowance → 24,
   YTickLabelAllowance → 29,

   FontSize → 25,
   LineThickness → 1
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
 ]
```

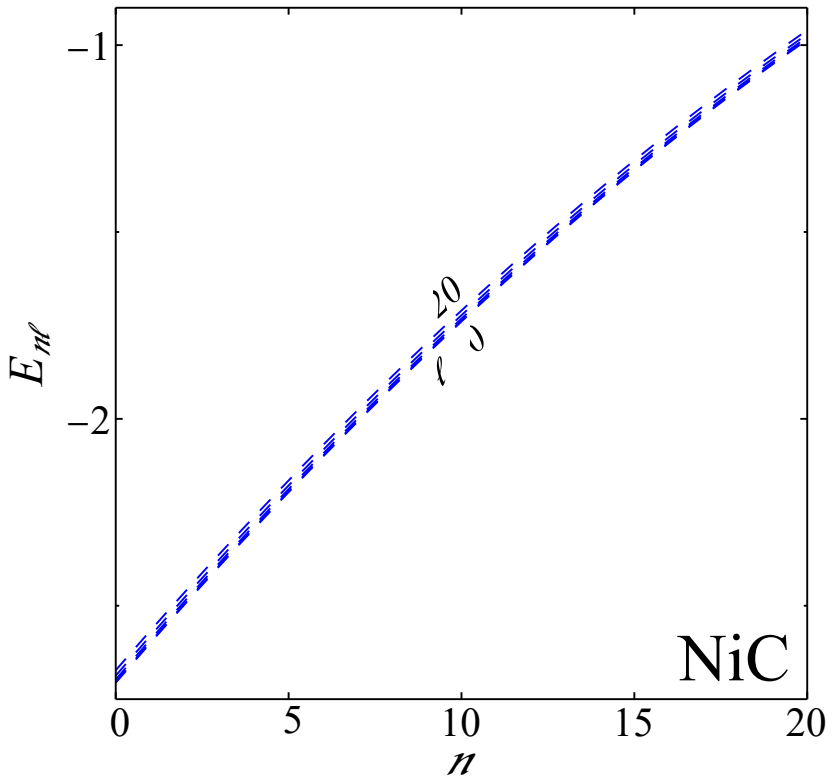
Out[•]=



NiC

In[•]:=
```
chooseMolecule["NiC"];
EnPlotNiC = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.895, 0.06}], "NiC", FontSize → 35];

    (*plots*)
    Do[
     FigLine[
      (*match x-
       y plot ranges here with down below. Needed for correct label positioning.*)
      Plot[E_n,ℓ, {n, 0, 20}, PlotRange → {Full, {-2.75, -0.9}}],
      (*the label of the lowest (ℓ=0) line is to the right, to reduce clutter.*)
      Which[ℓ == 0, RightLabel → textit[StringForm["ℓ=``", ℓ]],
       ℓ == 20, LeftLabel → textit[StringForm["ℓ=``", ℓ]],
       MemberQ[{5, 10, 15}, ℓ], LeftLabel → ""],
      (*positions adjusted so
       attached labels are roughly in the middle of the curves*)
      LeftLabelPosition → 0.5, RightLabelPosition → 0.5,
      FontSize → 20, LineColor → Blue, LineThickness → 1, LineDashing → 8
     ],
     {ℓ, 0, 20, 5}]
   },

   (*plot ranges*)
   XPlotRange → {0, 20}, XFrameLabel → textit["n"],
   YPlotRange → {-2.75, -0.9}, YFrameLabel → textit["E_n,ℓ"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 20, 5, 1],
   YTicks → LinTicks[-3, -0, 1, 2],
   (*to make space between ticks and axis labels*)
   XTickLabelAllowance → 24,
   YTickLabelAllowance → 29,

   FontSize → 25,
   LineThickness → 1
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
 ]
```

Out[•]=

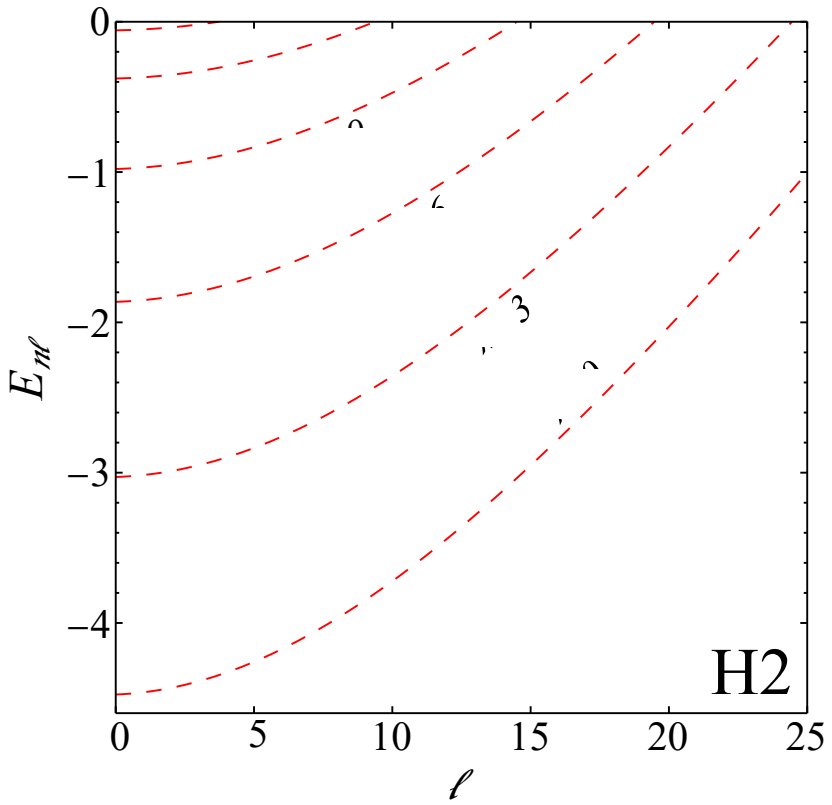


3. E_{nl} vs l

H_2

In[•]:=
```
chooseMolecule["H2"];
EℓPlotH2 = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.92, 0.06}], "H2", FontSize → 35];

    (*plots*)
    Do[
     FigLine[
      (*match x-
       y plot ranges here with down below. Needed for correct label positioning.*)
      Plot[Eₙℓ, {ℓ, 0, 25}, PlotRange → {Full, {-4.5, 0}}],
      (*the label of the lowest (ℓ=0) line is to the right, to reduce clutter.*)
      If[n ≠ 0, RightLabel → textit[StringForm["n=``", n]],
       LeftLabel → textit[StringForm["n=``", n]]],
      (*positions adjusted so
       attached labels are roughly in the middle of the curves*)
      LeftLabelPosition → 0.64, RightLabelPosition → 0.5,
      FontSize → 20, LineColor → Red, LineThickness → 1, LineDashing → 8
     ],
     {n, 0, 15, 3}]
   },

   (*plot ranges*)
   XPlotRange → {0, 25}, XFrameLabel → textit["ℓ"],
   YPlotRange → {-4.6, 0}, YFrameLabel → textit["Eₙℓ"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 25, 5, 1],
   YTicks → LinTicks[-4, 0, 1, 5],
   (*to make space between ticks and axis labels*)
   XTickLabelAllowance → 24,
   YTickLabelAllowance → 29,

   FontSize → 25,
   LineThickness → 1
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
 ]
```

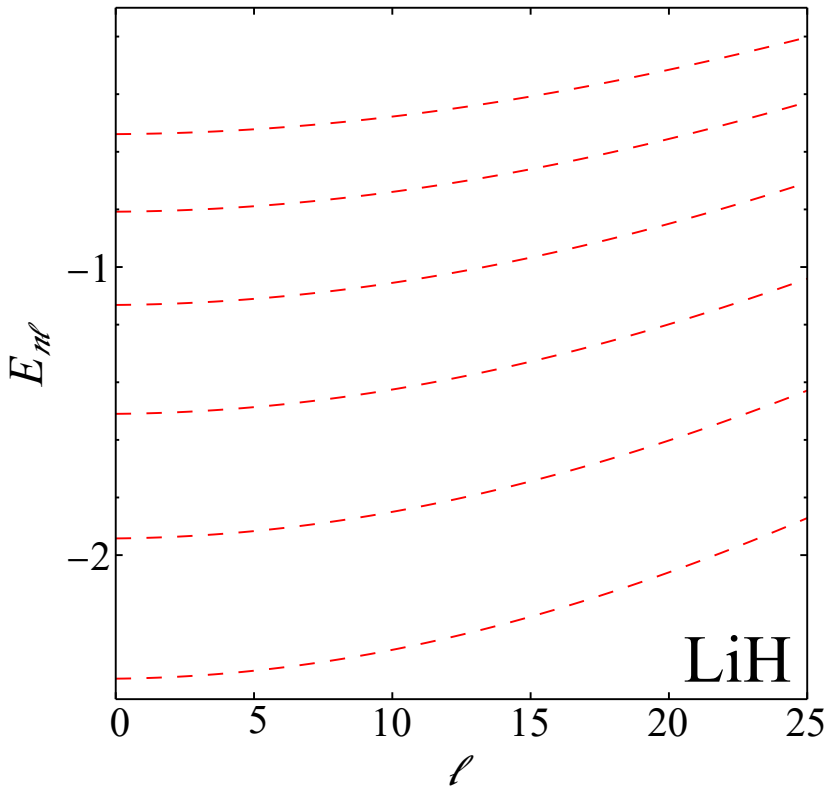
Out[•]=



LiH

In[ ]:=
```
chooseMolecule["LiH"];
EℓPlotLiH = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.9, 0.06}], "LiH", FontSize → 35];

    (*plots*)
    Do[
     FigLine[
      (*match x-
       y plot ranges here with down below. Needed for correct label positioning.*)
      Plot[E_{n,ℓ}, {ℓ, 0, 25}, PlotRange → {Full, {-2.5, -0.1}}],
      LeftLabel → textit[StringForm["n=``", n]],
      (*positions adjusted so
       attached labels are roughly in the middle of the curves*)
      LeftLabelPosition → 0.52,
      FontSize → 20, LineColor → Red, LineThickness → 1, LineDashing → 8
     ],
     {n, 0, 15, 3}]
   },

   (*plot ranges*)
   XPlotRange → {0, 25}, XFrameLabel → textit["ℓ"],
   YPlotRange → {-2.5, -0.1}, YFrameLabel → textit["E_{n,ℓ}"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 25, 5, 1],
   YTicks → LinTicks[-2, 0, 1, 5],
   (*to make space between ticks and axis labels*)
   XTickLabelAllowance → 24,
   YTickLabelAllowance → 29,

   FontSize → 25,
   LineThickness → 1
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
 ]
```

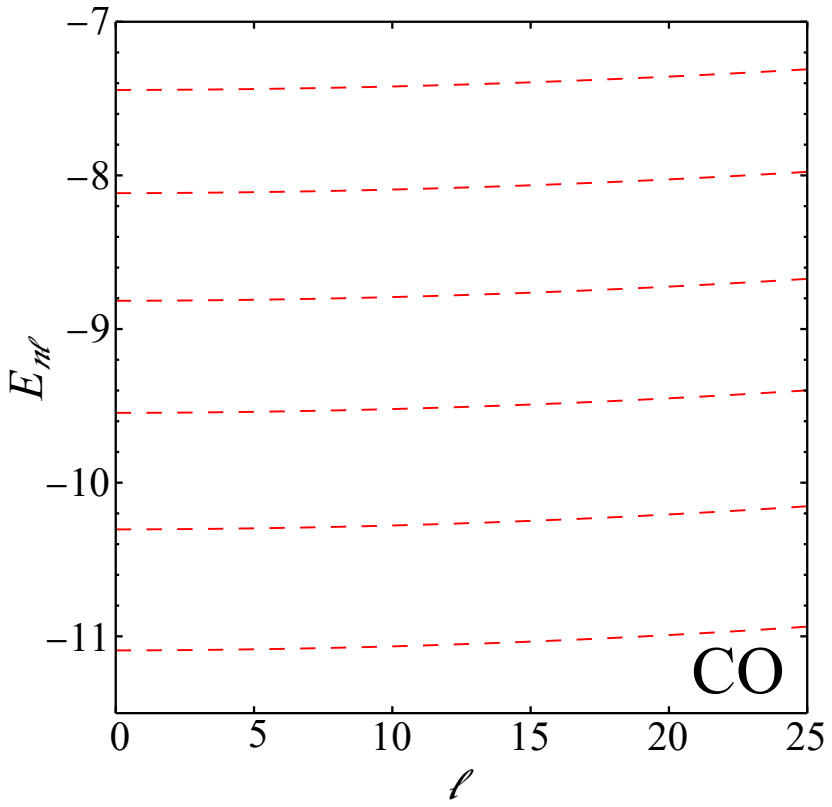
Out[•]=



CO

```
In[•]:= chooseMolecule["CO"];
        EℓPlotCO = Figure[
          FigurePanel[
           {
            (*label*)
            FigLabel[Scaled[{0.90, 0.06}], "CO", FontSize → 35];

            (*plots*)
            Do[
             FigLine[
              (*match x-
               y plot ranges here with down below. Needed for correct label positioning.*)
              Plot[E_{n,ℓ}, {ℓ, 0, 25}, PlotRange → {Full, {-11.5, -7}}],
              LeftLabel → textit[StringForm["n=``", n]],
              (*positions adjusted so
               attached labels are roughly in the middle of the curves*)
              LeftLabelPosition → 0.52,
              FontSize → 20, LineColor → Red, LineThickness → 1, LineDashing → 8
             ],
             {n, 0, 15, 3}]
           },

           (*plot ranges*)
           XPlotRange → {0, 25}, XFrameLabel → textit["ℓ"],
           YPlotRange → {-11.5, -7}, YFrameLabel → textit["E_{nℓ}"],

           (*ticks*)
           (*LinTicks[start, end, step, minor_ticks]*)
           XTicks → LinTicks[0, 25, 5, 1],
           YTicks → LinTicks[-11, -7, 1, 5],
           (*to make space between ticks and axis labels*)
           XTickLabelAllowance → 24,
           YTickLabelAllowance → 29,

           FontSize → 25,
           LineThickness → 1.2
          ],

          (*dimensions*)
          CanvasSize → {5, 5},
          (*margins*)
          (*{{left,right},{bottom,top}}*)
          CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
         ]
```

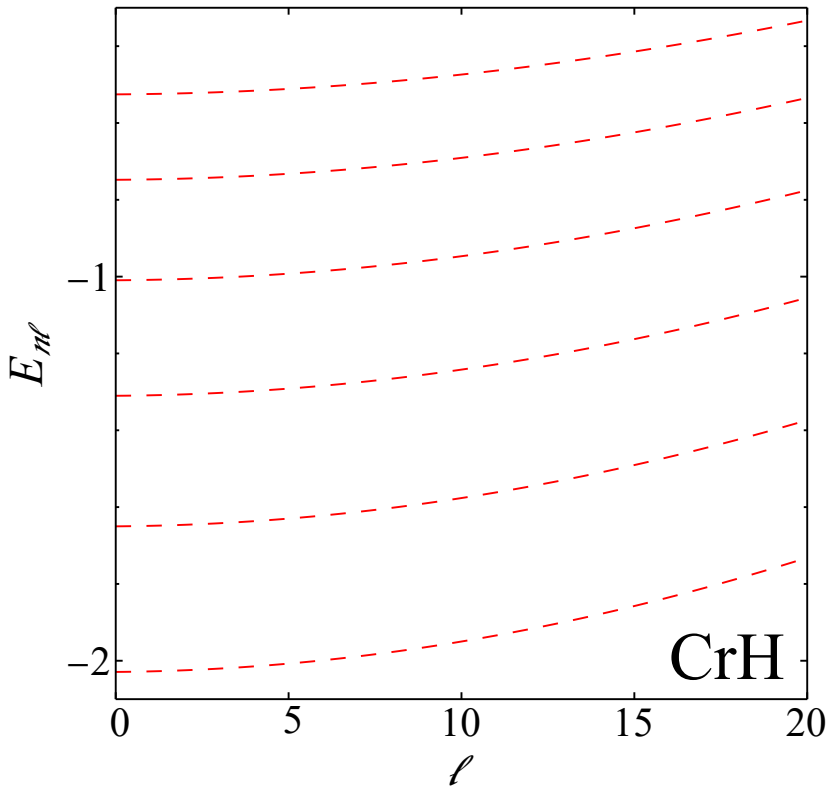
Out[•]=



CrH

In[•]:=
```
chooseMolecule["CrH"];
EℓPlotCrH = Figure[
  FigurePanel[
   {
    (*label*)
    FigLabel[Scaled[{0.885, 0.06}], "CrH", FontSize → 35];

    (*plots*)
    Do[
     FigLine[
      (*match x-
       y plot ranges here with down below. Needed for correct label positioning.*)
      Plot[E_{n,ℓ}, {ℓ, 0, 20}, PlotRange → {Full, {-2.1, -0.3}}],
      LeftLabel → textit[StringForm["n=``", n]],
      (*positions adjusted so
       attached labels are roughly in the middle of the curves*)
      LeftLabelPosition → 0.52,
      FontSize → 20, LineColor → Red, LineThickness → 1, LineDashing → 8
     ],
     {n, 0, 10, 2}]
   },

   (*plot ranges*)
   XPlotRange → {0, 20}, XFrameLabel → textit["ℓ"],
   YPlotRange → {-2.1, -0.3}, YFrameLabel → textit["E_{n,ℓ}"],

   (*ticks*)
   (*LinTicks[start, end, step, minor_ticks]*)
   XTicks → LinTicks[0, 20, 5, 1],
   YTicks → LinTicks[-2, 0, 1, 5],
   (*to make space between ticks and axis labels*)
   XTickLabelAllowance → 24,
   YTickLabelAllowance → 29,

   FontSize → 25,
   LineThickness → 1
  ],

  (*dimensions*)
  CanvasSize → {5, 5},
  (*margins*)
  (*{{left,right},{bottom,top}}*)
  CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
 ]
```

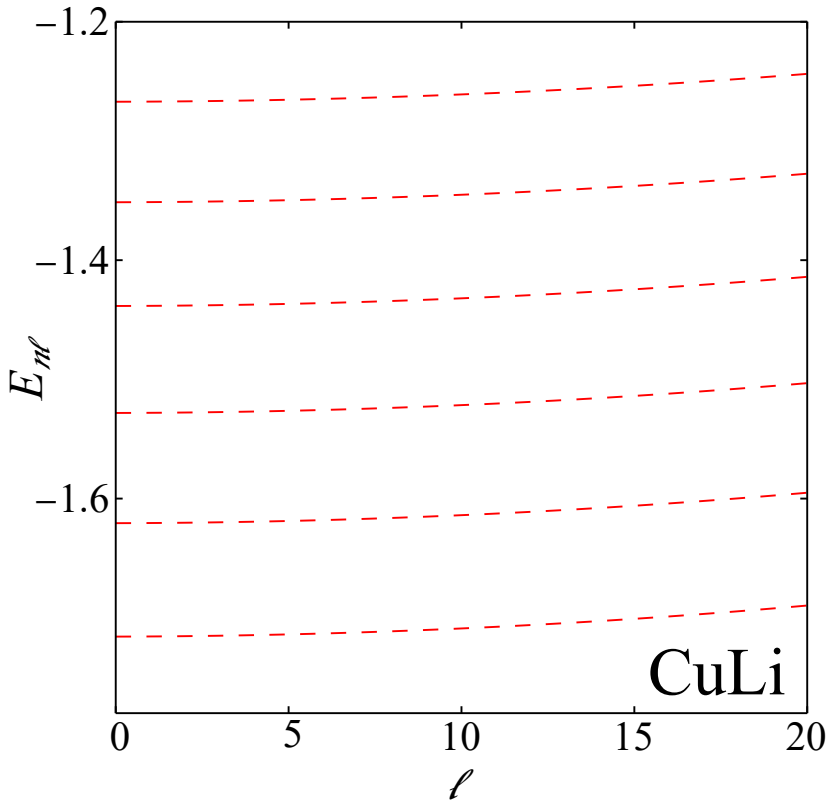
Out[•]=



CuLi

```
In[•]:= chooseMolecule["CuLi"];
        EℓPlotCuLi = Figure[
          FigurePanel[
           {
            (*label*)
            FigLabel[Scaled[{0.87, 0.06}], "CuLi", FontSize → 35];

            (*plots*)
            Do[
             FigLine[
              (*match x-
               y plot ranges here with down below. Needed for correct label positioning.*)
              Plot[E_{nℓ}, {ℓ, 0, 20}, PlotRange → {Full, {-1.78, -1.2}}],
              LeftLabel → textit[StringForm["n=``", n]],
              (*positions adjusted so
               attached labels are roughly in the middle of the curves*)
              LeftLabelPosition → 0.52,
              FontSize → 20, LineColor → Red, LineThickness → 1, LineDashing → 8
             ],
             {n, 0, 10, 2}]
           },

           (*plot ranges*)
           XPlotRange → {0, 20}, XFrameLabel → textit["ℓ"],
           YPlotRange → {-1.78, -1.2}, YFrameLabel → textit["E_{nℓ}"],

           (*ticks*)
           (*LinTicks[start, end, step, minor_ticks]*)
           XTicks → LinTicks[0, 20, 5, 1],
           YTicks → LinTicks[-1.8, -1.2, 0.2, 1],
           (*to make space between ticks and axis labels*)
           XTickLabelAllowance → 24,
           YTickLabelAllowance → 29,

           FontSize → 25,
           LineThickness → 1
          ],

          (*dimensions*)
          CanvasSize → {5, 5},
          (*margins*)
          (*{{left,right},{bottom,top}}*)
          CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
         ]
```

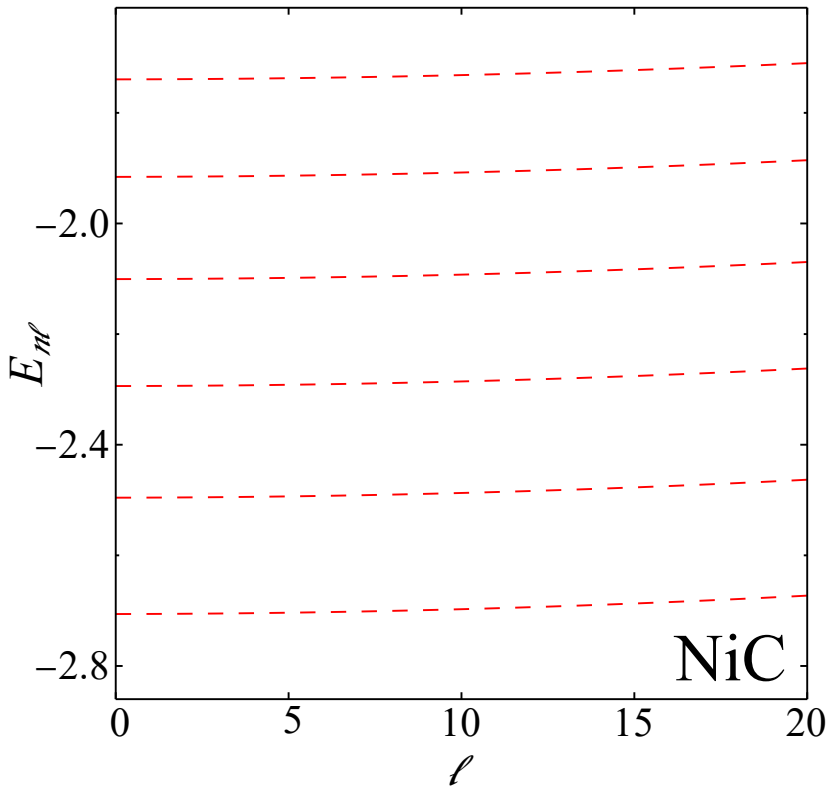
Out[•]=



NiC

```
In[•]:= chooseMolecule["NiC"];
        EℓPlotNiC = Figure[
          FigurePanel[
           {
            (*label*)
            FigLabel[Scaled[{0.89, 0.06}], "NiC", FontSize → 35];

            (*plots*)
            Do[
             FigLine[
              (*match x-
               y plot ranges here with down below. Needed for correct label positioning.*)
              Plot[E_nℓ, {ℓ, 0, 20}, PlotRange → {Full, {-2.86, -1.61}}],
              LeftLabel → textit[StringForm["n=``", n]],
              (*positions adjusted so
               attached labels are roughly in the middle of the curves*)
              LeftLabelPosition → 0.52,
              FontSize → 20, LineColor → Red, LineThickness → 1, LineDashing → 8
             ],
             {n, 0, 10, 2}]
           },

           (*plot ranges*)
           XPlotRange → {0, 20}, XFrameLabel → textit["ℓ"],
           YPlotRange → {-2.86, -1.61}, YFrameLabel → textit["E_nℓ"],

           (*ticks*)
           (*LinTicks[start, end, step, minor_ticks]*)
           XTicks → LinTicks[0, 20, 5, 1],
           YTicks → LinTicks[-2.8, -1.6, 0.4, 2],
           (*to make space between ticks and axis labels*)
           XTickLabelAllowance → 24,
           YTickLabelAllowance → 29,

           FontSize → 25,
           LineThickness → 1
          ],

          (*dimensions*)
          CanvasSize → {5, 5},
          (*margins*)
          (*{{left,right},{bottom,top}}*)
          CanvasMargin → {{0.85, 0.2}, {0.65, 0.2}}
         ]
```

Out[•]=

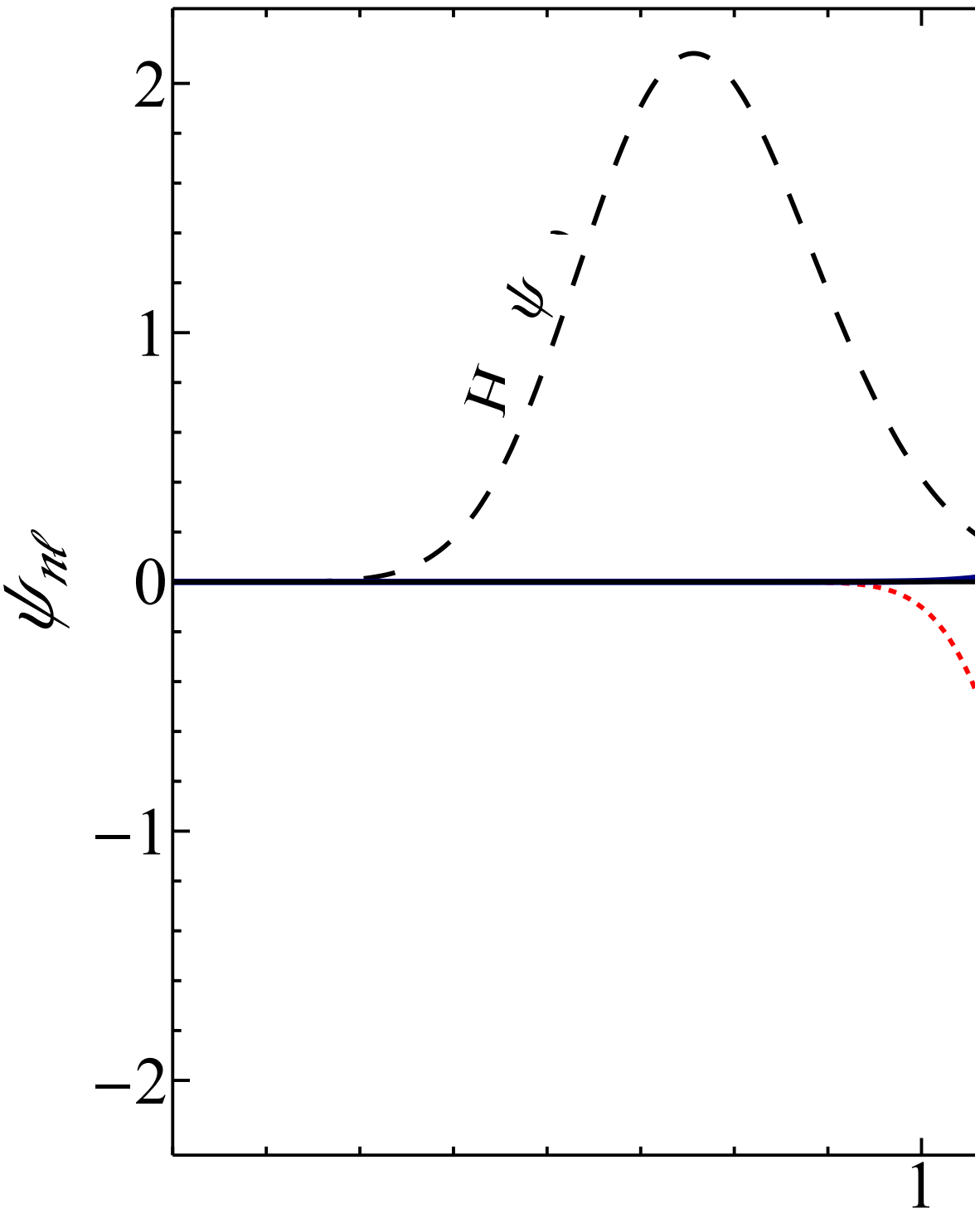


Wavefunctions

In[•]:=
```
wavefunctionsPlot = Figure[
  FigurePanel[
   {
    (*plots*)
    (*match x-y plot ranges in Plot[] with
      Scidraw settings below. Needed for correct label positioning.*)
    chooseMolecule["H2"]; n = 0; ℓ = 0;
    FigLine[
     Plot[Evaluate[ψ_{nℓ}[r]], {r, 0.2, 2.65}, PlotRange → {Full, {-2.3, 2.3}}],
     CenterLabel → StringForm["H2: ψ_{0,0}"],
     CenterLabelPosition → 0.18, TextOffset → Bottom,
     FontSize → 40, LineColor → Black, LineThickness → 3, LineDashing → 20
    ];

    chooseMolecule["HCl"]; n = 1; ℓ = 1;
    FigLine[
     Plot[Evaluate[ψ_{nℓ}[r]], {r, 0.2, 2.65}, PlotRange → {Full, {-2.3, 2.3}}],
     CenterLabel → StringForm["HCl: ψ_{1,1}"],
     CenterLabelPosition → 0.41, TextOffset → Top,
     FontSize → 40, LineColor → Red, LineThickness → 3, LineDashing → 5
    ];

    chooseMolecule["LiH"]; n = 2; ℓ = 0;
```

```
   FigLine[
    Plot[Evaluate[ψnℓ[r]], {r, 0.2, 2.65}, PlotRange → {Full, {-2.3, 2.3}}],
    CenterLabel → StringForm["LiH: ψ2,0"],
    CenterLabelPosition → 0.72, TextOffset → Bottom,
    FontSize → 40, LineColor → NavyBlue, LineThickness → 4, LineDashing → 0
   ];

   chooseMolecule["LiH"]; n = 2; ℓ = 15;
   FigLine[
    Plot[Evaluate[ψnℓ[r]], {r, 0.2, 2.65}, PlotRange → {Full, {-2.3, 2.3}}],
    CenterLabel → StringForm["LiH: ψ2,15"],
    CenterLabelPosition → 0.84, TextOffset → Bottom, FontSize → 40,
    LineColor → NavyBlue, LineThickness → 3, LineOpacity → 0.7, LineDashing → 8
   ];

   FigRule[Horizontal, 0, All, LineThickness → 3];
  },

  (*plot ranges*)
  XPlotRange → {0.2, 2.65}, XFrameLabel → textit["r (Å)"],
  YPlotRange → {-2.3, 2.3}, YFrameLabel → textit["ψnℓ"],

  (*ticks*)
  (*LinTicks[start, end, step, minor_ticks]*)
  XTicks → LinTicks[0, 3, 1, 10],
  YTicks → LinTicks[-2, 2, 1, 5],
  (*to make space between ticks and axis labels*)
  XTickLabelAllowance → 40,
  YTickLabelAllowance → 60,

  FontSize → 50,
  LineThickness → 2
 ],

 (*dimensions*)
 CanvasSize → {20, 10},
 (*margins*)
 (*{{left,right},{bottom,top}}*)
 CanvasMargin → {{1.7, 0.5}, {1.3, 0.4}}
]
```

Out[•]=



In[•]:=
```
(*to open the plot in a new window*)
(*CreateDocument[Dynamic[wavefunctionsPlot],WindowSize→{500,500}];*)
```

Misc

In[•]:=
```
(*saving plots*)
(*potentialPlotList=
 {potentialPlotH2,potentialPlotLiH,potentialPlotHCl,potentialPlotCO};
Do[Export[ToString[StringForm["plots/potentialPlots/``.pdf",moleculesList[[i]]],
  potentialPlotList[[i]],{i,1,Length[potentialPlotList]}]
*)
plotMoleculesList = {"H2", "LiH", "CO", "CrH", "CuLi", "NiC"};
EnPlotList = {EnPlotH2, EnPlotLiH, EnPlotCO, EnPlotCrH, EnPlotCuLi, EnPlotNiC};
ElPlotList = {ElPlotH2, ElPlotLiH, ElPlotCO, ElPlotCrH, ElPlotCuLi, ElPlotNiC};

Do[
 Export[ToString[StringForm["plots/E_vs_n/``.png", plotMoleculesList[[i]]],
  EnPlotList[[i]], ImageResolution → 500];
 Export[ToString[StringForm["plots/E_vs_l/``.png", plotMoleculesList[[i]]],
  ElPlotList[[i]], ImageResolution → 500];

 , {i, 1, Length[plotMoleculesList]}]
```