Zadanie 2

Projektowanie struktur półprzewodnikowych.

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```
PlotlyJSBackend()
```

```
interpolation (generic function with 2 methods)
```

```
interpolation(x, q_A, q_B, C=0) = x * q_A + (1 - x) * q_B + x * (1 - x) * C
```

```
unknown_mass_CsSiI₃ = 0.082
```

```
unknown_mass_CsSiI₃ = 0.5 * (0.095 + 0.069) # średnia z CsXI₃
```

```
CsPbI₃ =
  (Eg = 1.73, Δ = 1.44, γ₁ = 9.1, γ₂ = 3.6, γ₃ = 0.7, mₕ = 0.095, Ep = 41.6, a = 6.238)
```

```
CsPbI₃ = @NamedTuple{Eg, Δ, γ₁, γ₂, γ₃, mₕ, Ep, a}((
    1.73, # Eg
    1.44, # Δ
    9.1, # γ₁
    3.6, # γ₂
    0.7, # γ₃
    0.095, # mₕ
    41.6, # Ep
    6.238 # a
))
```

```
CsSiI₃ =
  (Eg = 0.31, Δ = 0.5, γ₁ = 24.3, γ₂ = 11.5, γ₃ = 8.1, mₕ = 0.082, Ep = 18.9, a = 5.892)
```

```
CsSiI₃ = @NamedTuple{Eg, Δ, γ₁, γ₂, γ₃, mₕ, Ep, a}((
    0.31, # Eg
    0.50, # Δ
    24.3, # γ₁
    11.5, # γ₂
    8.1, # γ₃
    unknown_mass_CsSiI₃, # mₕ
    18.9, # Ep
    5.892 # a
))
```

```
CsPbₓSi₁-ₓI₃ (generic function with 2 methods)
```

```
CsPbₓSi₁-ₓI₃(x,C=0) = @NamedTuple{Eg, Δ, γ₁, γ₂, γ₃, mₕ, Ep, a}(
    interpolation.(x, collect(CsPbI₃), collect(CsSiI₃), C)
)
```

```
xs = 0.0:0.01:1.0
```

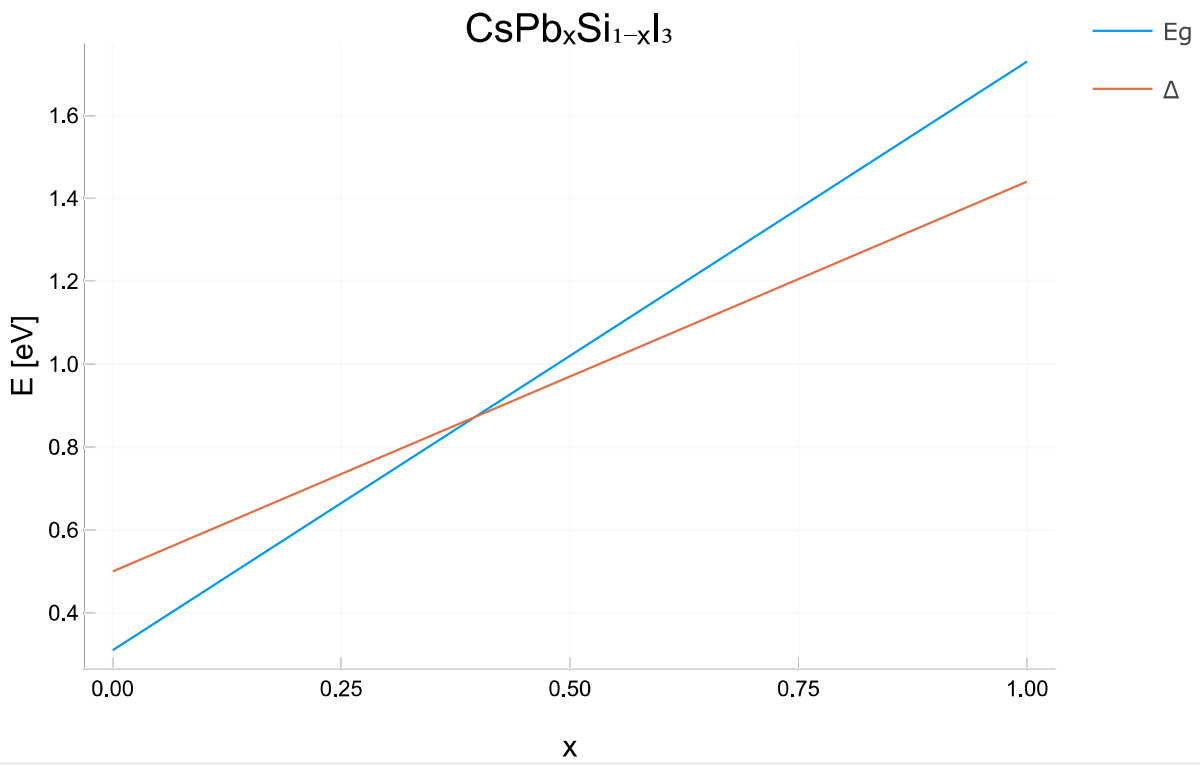
```
xs = 0:0.01:1
```

```
ys =
```

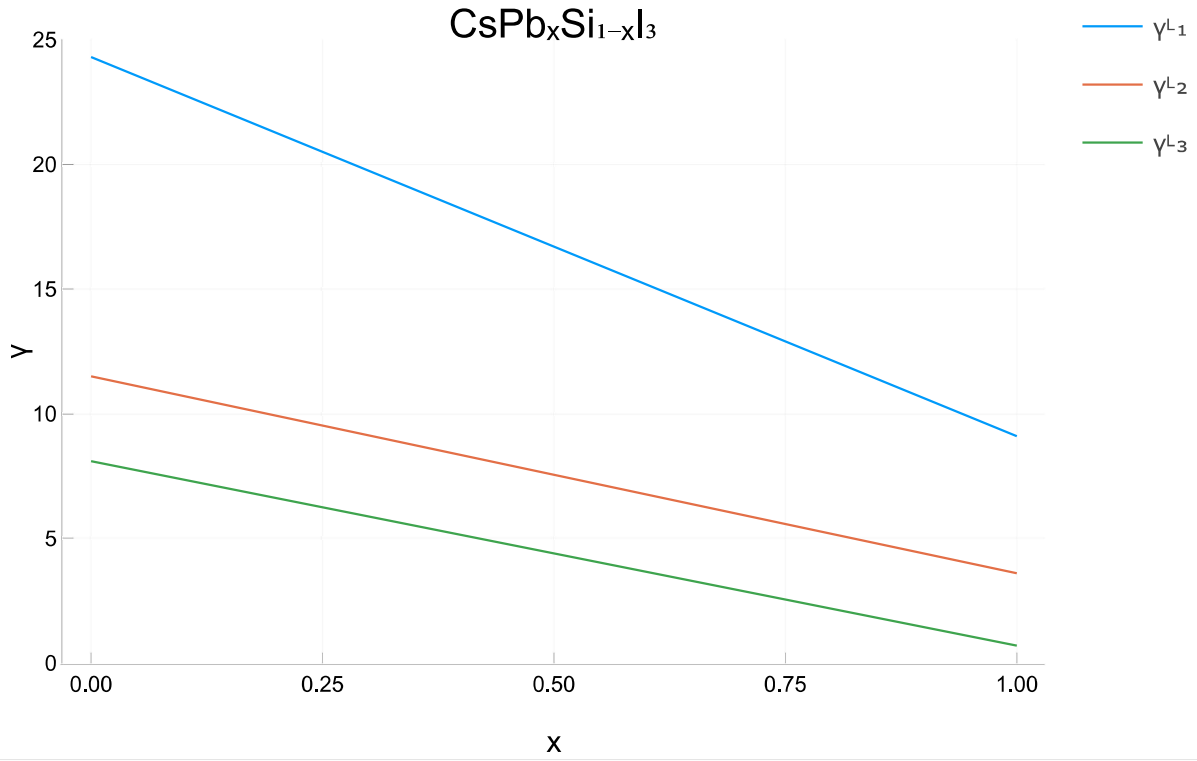

```
[(Eg = 0.31, Δ = 0.5, γ₁ = 24.3, γ₂ = 11.5, γ₃ = 8.1, mₕ = 0.082, Ep = 18.9, a = 5.892), (
```


```
ys = CsPbₓSi₁-ₓI₃.(xs)
```

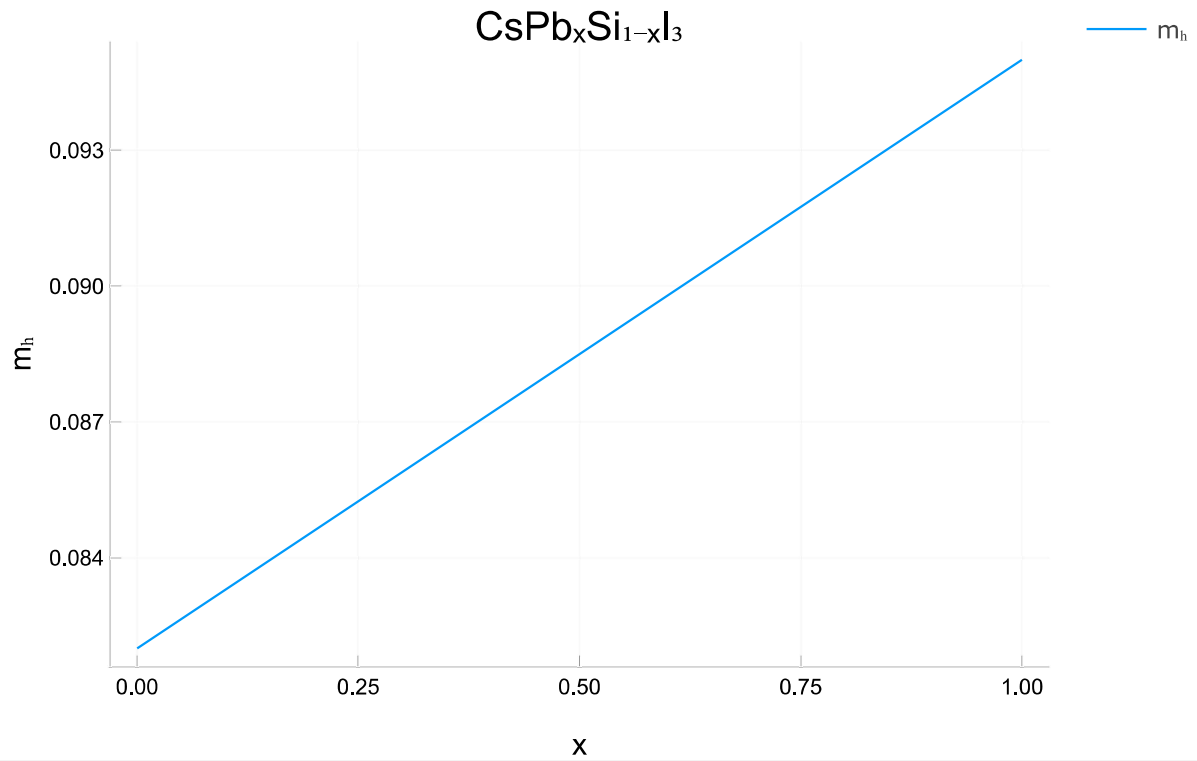
Without bowing



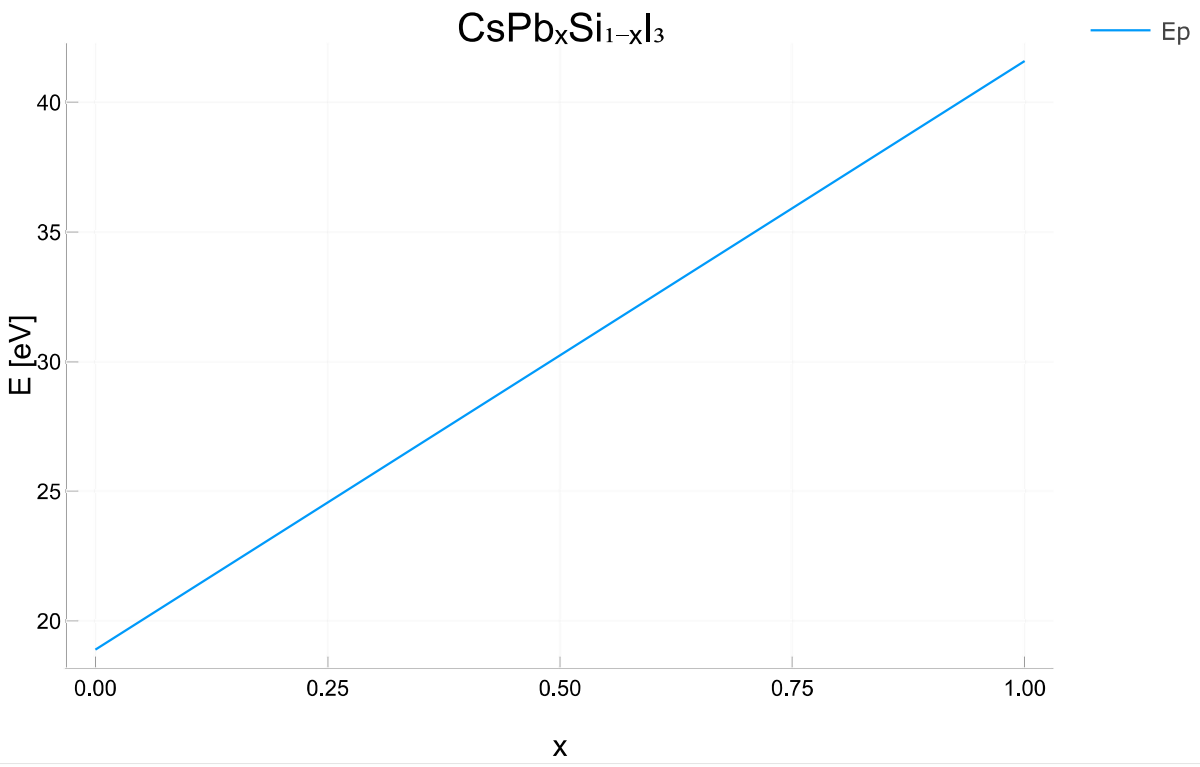

```
plot(xs, [y[E] for y in ys, E in [:Eg, :Δ]],
    xlabel=:x, ylabel="E [eV]", title=:CsPbₓSi₁-ₓI₃, labels=["Eg" "Δ"])
```



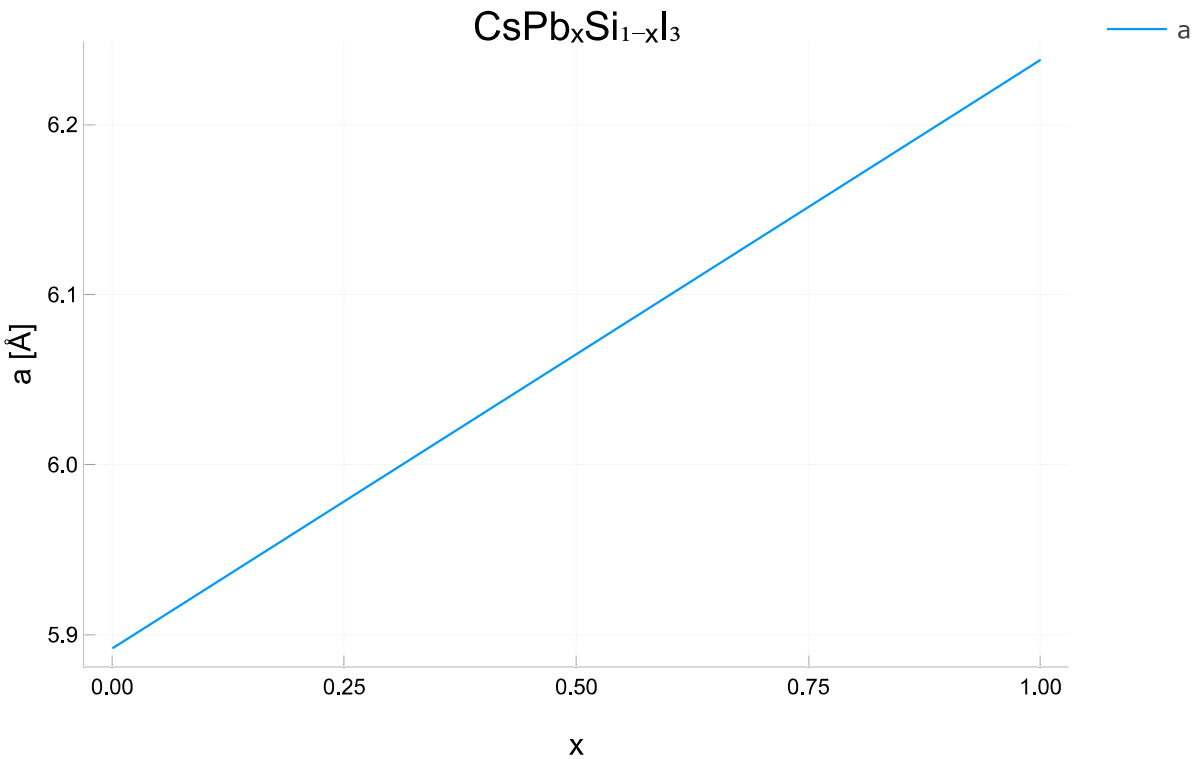

```
plot(xs, [y[gamma] for y in ys, gamma in [:γ₁, :γ₂, :γ₃]],
    xlabel=:x, ylabel=:γ, title=:CsPbₓSi₁₋ₓI₃, label=["γᴸ₁" "γᴸ₂" "γᴸ₃"])
```



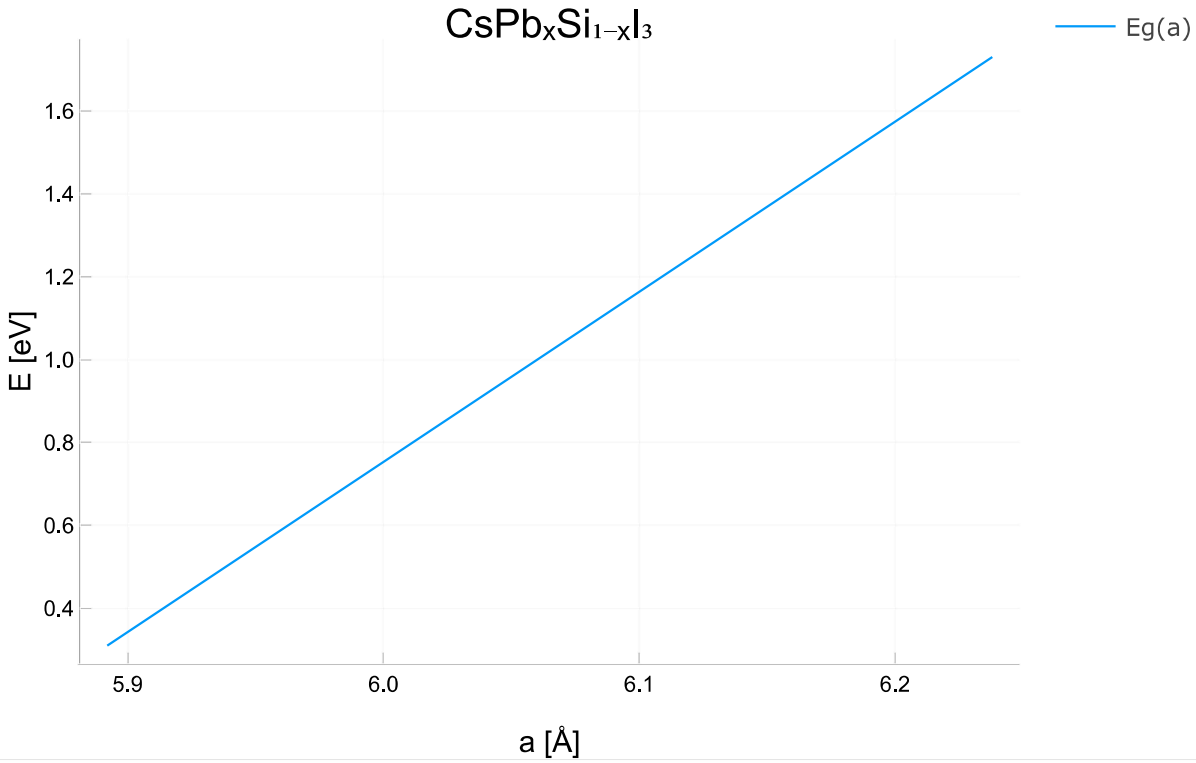

```
plot(xs, [y.mₕ for y in ys],
    xlabel=:x, ylabel="mₕ", title=:CsPbₓSi₁₋ₓI₃, label="mₕ")
```




```
plot(xs, [y.Ep for y in ys],
    xlabel=:x, ylabel="E [eV]", title=:CsPbₓSi₁₋ₓI₃, label="Ep")
```




```
plot(xs, [y.a for y in ys],
    xlabel=:x, ylabel="a [Å]", title=:CsPbₓSi₁₋ₓI₃, label="a")
```

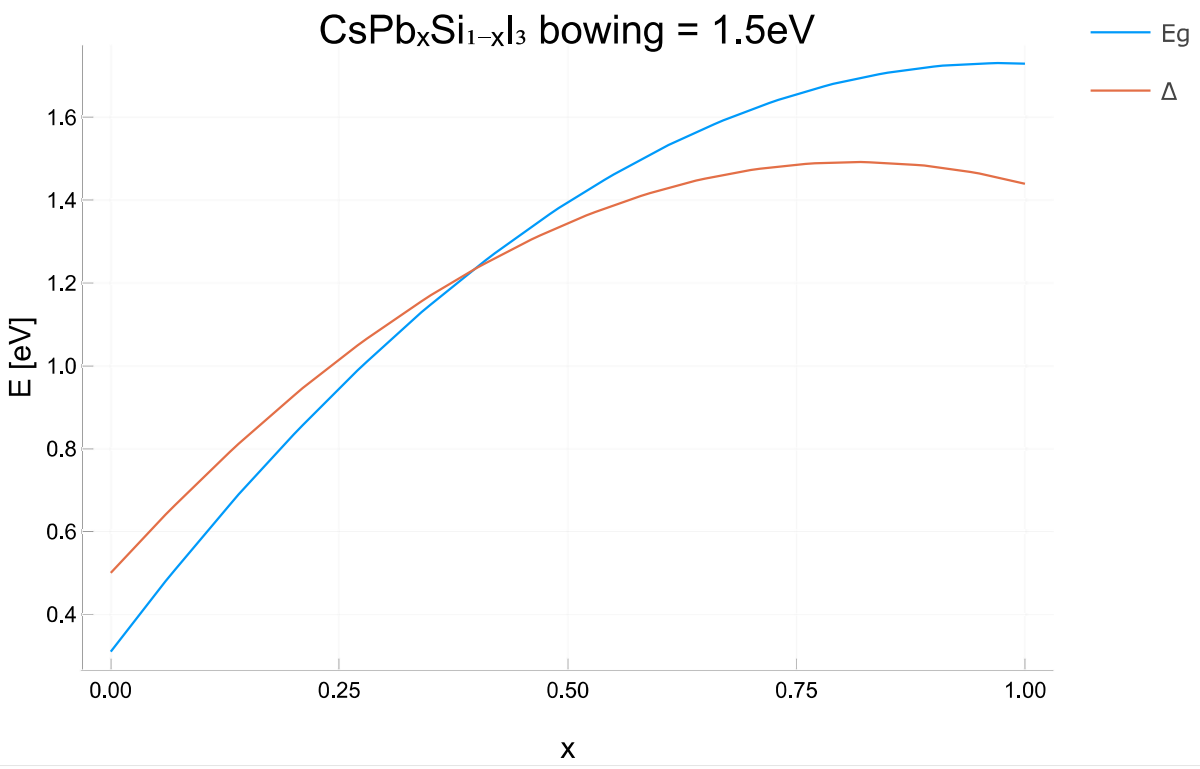



```
plot([y.a for y in ys], [y.Eg for y in ys],
    xlabel="a [Å]", ylabel="E [eV]", title=:CsPbₓSi₁-ₓI₃, label="Eg(a)")
```

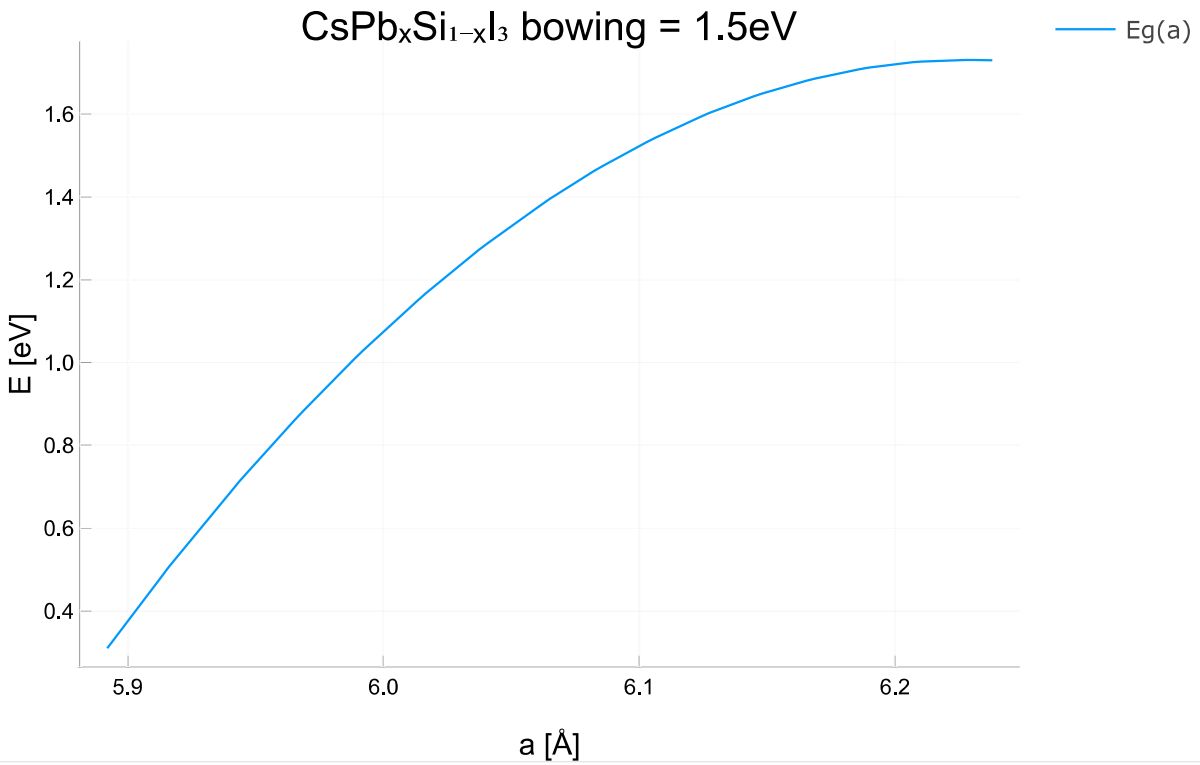
With bowing C = 1.5

```
ysb15 =
  [(Eg = 0.31, Δ = 0.5, γ₁ = 24.3, γ₂ = 11.5, γ₃ = 8.1, mₕ = 0.082, Ep = 18.9, a = 5.892), (
```

```
ysb15 = CsPbₓSi₁-ₓI₃.(xs, 1.5)
```




```
plot(xs, [y[E] for y in ysb15, E in [:Eg, :Δ]],
    xlabel=:x, ylabel="E [eV]", title="CsPbₓSi₁₋ₓI₃ bowing = 1.5eV", labels=["Eg" "Δ"])
```




```
plot([y.a for y in ys], [y.Eg for y in ysb15],
    xlabel="a [Å]", ylabel="E [eV]", title="CsPbₓSi₁₋ₓI₃ bowing = 1.5eV", label="Eg(a)")
```