Zadanie 4

Michał Łukomski 255552

```
PlotlyJSBackend()
```

```
interpolation (generic function with 4 methods)
```

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

    function interpolation(x, q_A::Dict, q_B::Dict, C=0)
        @assert keys(q_A) == keys(q_B)
        res = Dict()
        for (key, v_A) in q_A
            v_B = q_B[key]
            res[key] = interpolation(x, v_A, v_B, C)
        end
        return res
    end
end
```

```
Dict("Eg" ⇒ 0.31, "Δ" ⇒ 0.5, "γ₁" ⇒ 24.3, "γ₃" ⇒ 8.1, "γ₂" ⇒ 11.5, "α" ⇒ 0.1, "mₕ" =
```

```julia
begin
    unknown_mass_CsSiI3 = 0.5 * (0.095 + 0.069)
    CsPbI₃ = Dict(zip(["Eg", "Δ", "γ₁", "γ₂", "γ₃", "mₕ", "Ep", "a", "α"], [
        1.73, # Eg eV
        1.44, # Δ
        9.1, # γ₁
        3.6, # γ₂
        0.7, # γ₃
        0.095, # mₕ
        41.6, # Ep
        6.238, # a
        0.9, # α meV/K
    ]))

    CsSiI₃ = Dict(zip(["Eg", "Δ", "γ₁", "γ₂", "γ₃", "mₕ", "Ep", "a", "α"], [
        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
        0.1, # α meV/K
    ]))
end
```

```
0.24733333333333332
```

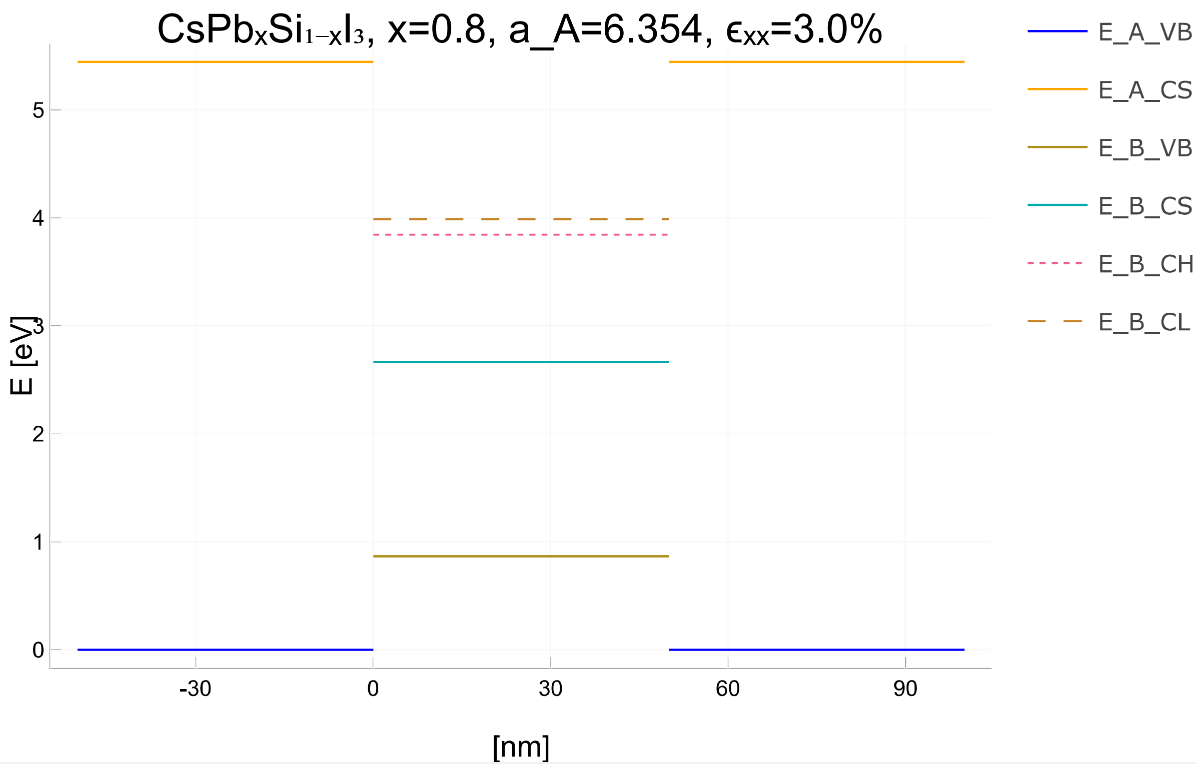
```julia
begin
    # https://www.sciencedirect.com/science/article/pii/S003040261631021X?casa_token=o33T8v5jN3QAAAAA:I8IBYsFMKtk-aXxKz1GThGbgQfDKschBqnRRVHBQsx-ikcQH4iS-iVlYZ3DO8YZtA5JtWPR9eBo
    CsPbI₃["c₁₁"] = 34.405 # GPa
    CsPbI₃["c₁₂"] = 4.709 # GPa

    CsPbI₃["aᵛ"] = -2.762 # eV
    CsPbI₃["aᶜ"] = -0.177 # eV

    # CsSiI₃[val] = 1/3 ( CsPbI₃ + CsSnI₃ + CsGeI₃)
    # https://www.worldscientific.com/doi/abs/10.1142/S0217984921500561 - CsSiI₃
    # https://www.mdpi.com/2076-3417/10/15/5055 - CsGeI₃
    CsSiI₃["c₁₁"] = (CsPbI₃["c₁₁"] + 41.31 + 60.07) / 3
    CsSiI₃["c₁₂"] = (CsPbI₃["c₁₂"] + 3.69 + 48.61) / 3

    CsSiI₃["aᵛ"] = (CsPbI₃["aᵛ"] + -3.651 + -2.257) / 3
    CsSiI₃["aᶜ"] = (CsPbI₃["aᶜ"] + -0.052 + 0.971) / 3

end
```

```
plot_energy_diagram_AB (generic function with 1 method)
```

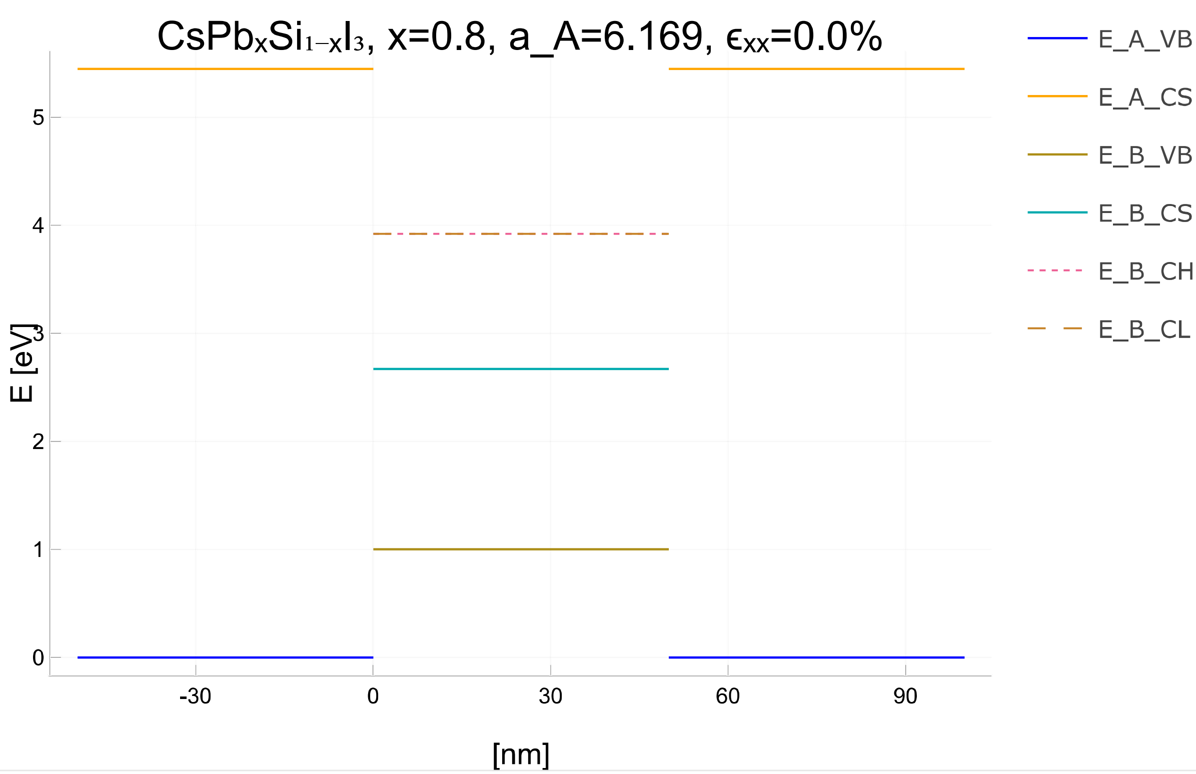
```julia
function plot_energy_diagram_AB(x, percentage)
    b = -2 # like GaAs
    T = 300 # K

    mat_B = interpolation(x, CsPbI₃, CsSiI₃)
    mat_B["EgT"] = mat_B["Eg"] + mat_B["α"] * 1e-3 * T

    a_A = mat_B["a"] * (1 + percentage)
    ϵₓₓ = (a_A - mat_B["a"]) / mat_B["a"]

    δE_Hᵛ = 2 * mat_B["aᵛ"] * (1 - mat_B["c₁₂"] / mat_B["c₁₁"]) * ϵₓₓ
    δE_Hᶜ = 2 * mat_B["aᶜ"] * (1 - mat_B["c₁₂"] / mat_B["c₁₁"]) * ϵₓₓ
    δE_S = b * (1 + mat_B["c₁₂"] / mat_B["c₁₁"]) * ϵₓₓ

    VBO_A = 0 # eV
    VBO_B = 1 # eV
    Eg_A = VBO_B + mat_B["Eg"] + 3 # eV

    VB_B = VBO_B
    CS_B = VBO_B + mat_B["EgT"]
    CH_B = VBO_B + mat_B["EgT"] + mat_B["Δ"]
    CL_B = CH_B

    VB_A = VBO_A
    CS_A = VBO_A + Eg_A

    E_VB = VB_B .+ δE_Hᵛ
    E_CS = CS_B .+ δE_Hᶜ
    E_CH = CH_B .+ δE_Hᶜ .+ δE_S
    E_CL = CL_B .+ δE_Hᶜ .- δE_S

    d = 50 # nm
    X_A = vcat(-d:0, d:2d)
    X_B = 0:d

    fig = plot(-d:0, ones(d + 1) * VB_A, color=:blue, label="E_A_VB")
    plot!(fig, d:2d, ones(d + 1) * VB_A, color=:blue, label=:none)

    plot!(fig, -d:0, ones(d + 1) * CS_A, color=:orange, label="E_A_CS")
    plot!(fig, d:2d, ones(d + 1) * CS_A, color=:orange, label=:none)

    plot!(fig, 0:d, ones(d + 1) * E_VB, label="E_B_VB")
    plot!(fig, 0:d, ones(d + 1) * E_CS, label="E_B_CS")
    plot!(fig, 0:d, ones(d + 1) * E_CH, label="E_B_CH", linestyle=:dot)
    plot!(fig, 0:d, ones(d + 1) * E_CL, label="E_B_CL", linestyle=:dash)

    title!(fig, "CsPbₓSi₁₋ₓI₃, x=$x, a_A=$(round(a_A,digits=3)), ϵₓₓ=$(round(ϵₓₓ*100,digits=3))%")
    xlabel!(fig, "[nm]")
    ylabel!(fig, "E [eV]")
    return fig
end
```

Wykresy

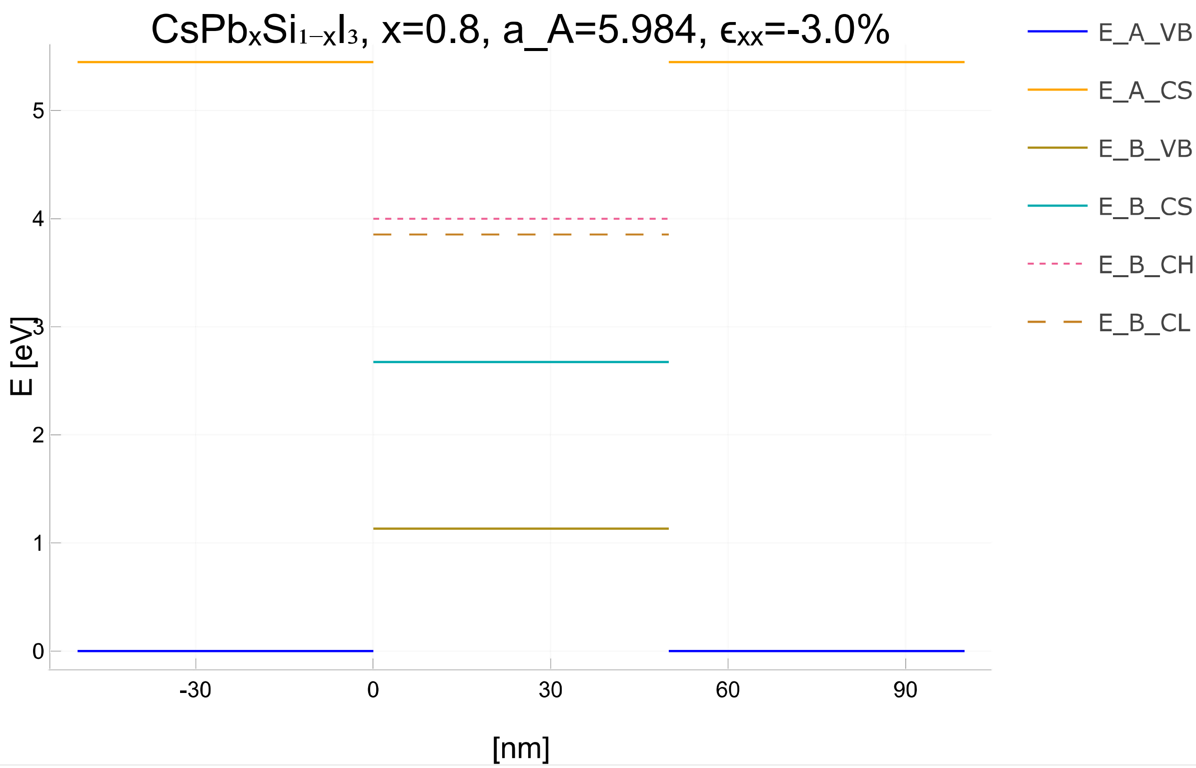
x = 0.8




```
plot_energy_diagram_AB(0.8, 0.03)
```

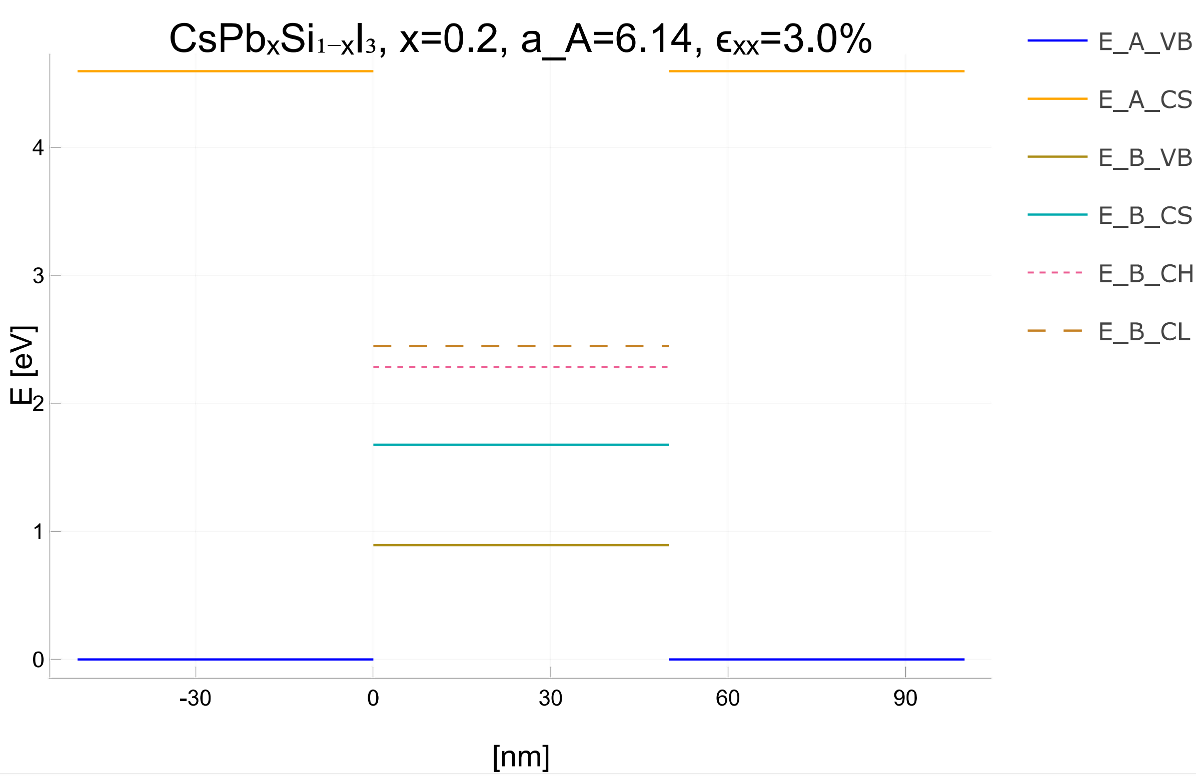



```
plot_energy_diagram_AB(0.8, 0.0)
```

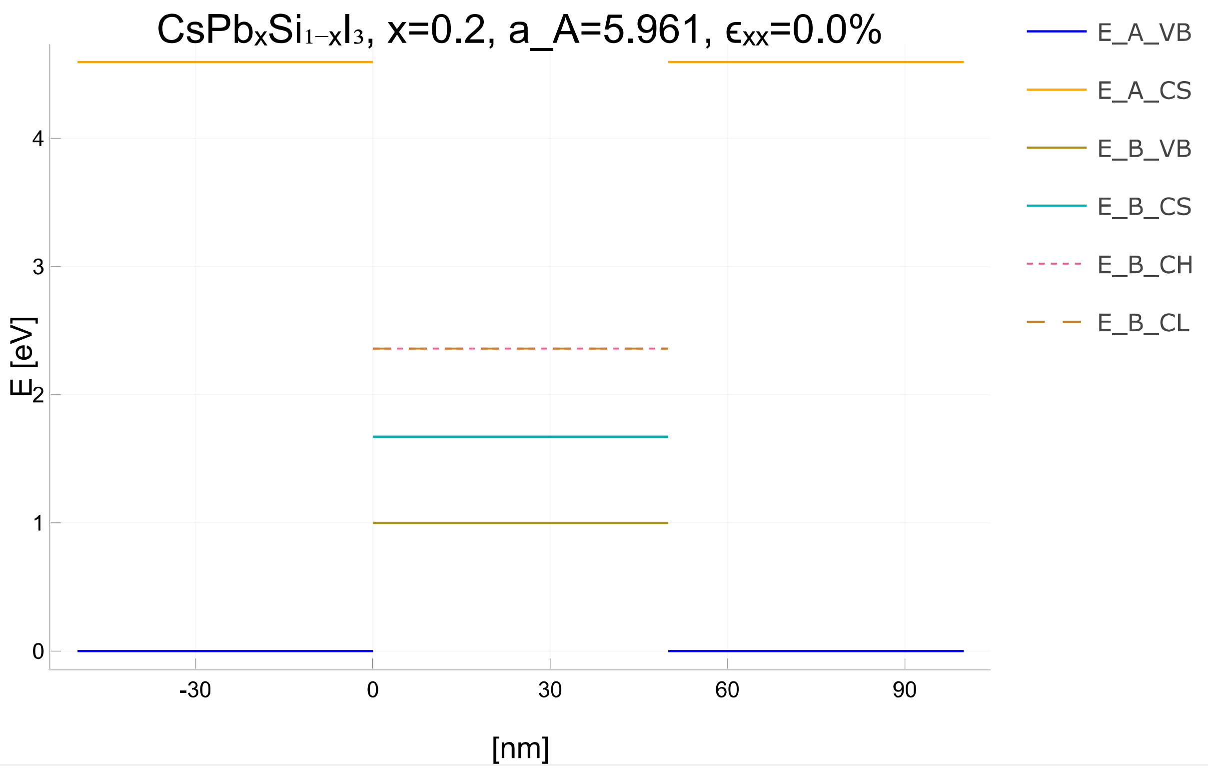



```
plot_energy_diagram_AB(0.8, -0.03)
```

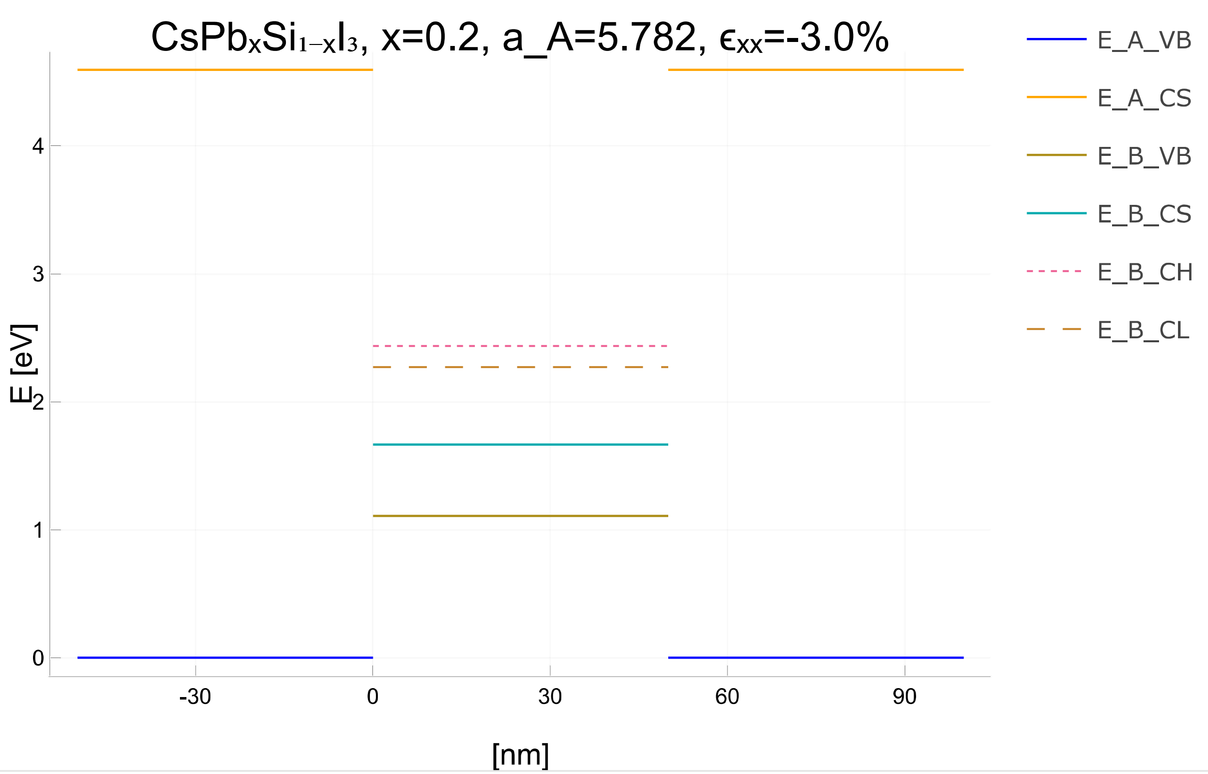
x = 0.2




```
plot_energy_diagram_AB(0.2, 0.03)
```




```
plot_energy_diagram_AB(0.2, 0.0)
```




```
plot_energy_diagram_AB(0.2, -0.03)
```