Supporting Information for *"[article title]"*

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Abstract

This Supporting Information includes:

[Use this section to include additional explanatory text such as an extended technical description of results, full details of mathematical models, etc.]

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Authorea documents are more than just text and figures. Every Authorea document is a Git repository that can host data, source code, or link to **datasets** and containers hosted elsewhere. You can add data specific to a figure/table by adding a figure to an article and then clicking on the figure. The menu that opens allows uploading **datasets** or link to external repositories.

Interactive elements such as interactive figures, executable codes, 3D CAD models, and every object linked to an html/jvs code can be included. Interactive elements can be added by clicking on **Insert -> Interactive Figure (fig).**

See the sections below for an overview of the possibilities that Authorea documents offer. Feel free to edit/remove/add sections as required, explore all the possibilities!

Equations

Equations can be inserted via **Insert -> Equation.** In this case Dirac equation. Typed in `LaTeX`.

Code

Code blocks can be inserted via **Insert -> Code Block.**

Some code in **markdown**, from (Hanwell et al., 2020):


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```


Tables

Tables can be inserted via **Insert -> Table.** Corresponding data can be linked to the table and either hosted locally or in an outside repository, using the 'Data Link' capability.

	DoF	wMUE	AIC	VCC	CVC	AVG ranking	Ref
DSD-PBEP86-D3(BJ)	7	2.14	2.29 (1)	3.61 (1)	2.3 (1)	1	54
PWPB95-D3(BJ)	10	2.69	2.97 (2)	4.99 (2)	2.85 (2)	2	34;55
B2PLYP-D3(BJ)	5	3.33	3.5 (3)	5.21 (3)	3.47 (3)	3	55;56
wB97M-V	12	3.43	3.87 (4)	6.76 (5)	3.76 (4)	4.33	57
PW6B95-D3(BJ)	9	3.75	4.11 (5)	6.76 (4)	3.98 (5)	4.67	58;59
PW6B95	6	5.27	5.6 (6)	8.58 (9)	5.43 (8)	7.67	59
PBE0-D3(BJ)	4	5.45	5.68 (7)	8.19 (8)	5.53 (9)	8	58;60
HSE-HJS	1	5.7	5.75 (9)	7.23 (6)	5.73 (15)	10	61;62
B3LYP-D3(BJ)	6	5.42	5.76 (10)	8.82 (11)	5.63 (13)	11.33	43;46;58;63;64;65
B97M-rV	12	5.05	5.69 (8)	9.93 (16)	5.53 (10)	11.33	66;67
PBE0	1	5.74	5.79 (12)	7.28 (7)	5.76 (16)	11.67	60
B97M-V	12	5.12	5.77 (11)	10.07 (17)	5.61 (11)	13	68;69
wB97X-V	10	5.33	5.89 (13)	9.89 (15)	5.7 (14)	14	70
SCAN-D3(BJ)	2	6.32	6.45 (14)	8.58 (10)	6.35 (24)	16	21;58
M06-2X	29	4.86	6.5 (15)	14.37 (34)	5.36 (7)	18.67	26
revPBE-D3(BJ)	4	6.49	6.76 (17)	9.74 (14)	6.6 (26)	19	58;71
B97-1	10	5.95	6.58 (16)	11.05 (21)	6.34 (23)	20	72
M05	22	5.47	6.82 (19)	13.84 (29)	6.1 (18)	22	22
M05-2X	19	5.82	7.05 (20)	13.74 (28)	6.26 (19)	22.33	23
MN15	59	3.68	6.76 (18)	20.16 (44)	5.35 (6)	22.67	32
BMK	17	6.04	7.16 (23)	13.57 (27)	6.27 (20)	23.33	73
M06-2X-D3(0)	35	5.03	7.16 (22)	16.89 (38)	5.62 (12)	24	26;74
PBE	1	7.41	7.48 (25)	9.39 (12)	7.43 (35)	24	20
revTPSS-D3(BJ)	6	6.76	7.17 (24)	10.99 (20)	6.99 (31)	25	58;75
N12-SX	26	5.51	7.15 (21)	15.26 (37)	5.97 (17)	25	30
PW91	1	7.56	7.64 (28)	9.59 (13)	7.58 (37)	26	76;77
t-HCTHh	17	6.36	7.54 (26)	14.28 (32)	6.98 (30)	29.33	78
TPSSh	1	8.04	8.12 (33)	10.2 (18)	8.07 (41)	30.67	79
PBE-D3(BJ)	3	7.81	8.05 (31)	11.19 (23)	7.87 (39)	31	20;58
B97-D3(0)	9	7.23	7.91 (30)	13.02 (26)	7.61 (38)	31.33	58;75
M06-D3(0)	39	5.09	7.56 (27)	18.58 (41)	6.63 (27)	31.67	26;58
B3PW91	3	7.82	8.06 (32)	11.2 (24)	7.9 (40)	32	46;63;76;77
M06	33	5.58	7.78 (29)	17.98 (40)	6.85 (29)	32.67	26
TPSS	1	8.39	8.48 (37)	10.64 (19)	8.43 (44)	33.33	78
M11-D3(BJ)	46	5.18	8.28 (34)	21.81 (49)	6.29 (22)	35	68;79
M08-HX	47	5.24	8.46 (36)	22.5 (50)	6.29 (21)	35.67	27
revTPSS	1	8.79	8.88 (39)	11.15 (22)	8.83 (47)	36	75
M11	40	5.6	8.4 (35)	20.86 (46)	6.64 (28)	36.33	79

Videos

Videos can be included via **Insert -> Rich Media.** A screenshot of the video is used as corresponding static image in the exported PDF.

Rich media available at https://youtu.be/3vmQTbCjKNU

Interactive Figures

Interactive figure can be included via **Insert -> Interactive Figure (html)** [detailed guideline].

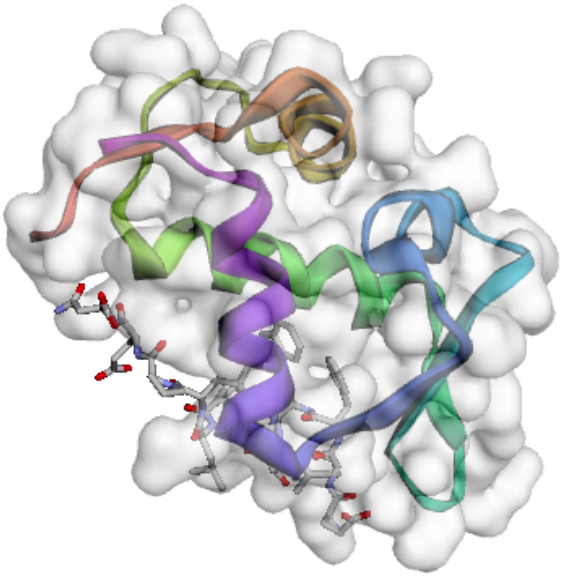

Figure 1: You may insert an Interactive version of the figures in the manuscript in the smart supporting information. The example here is created by 3Dmol.js figure. Data (In this case protein structure) available via the Data Link badge on the left.

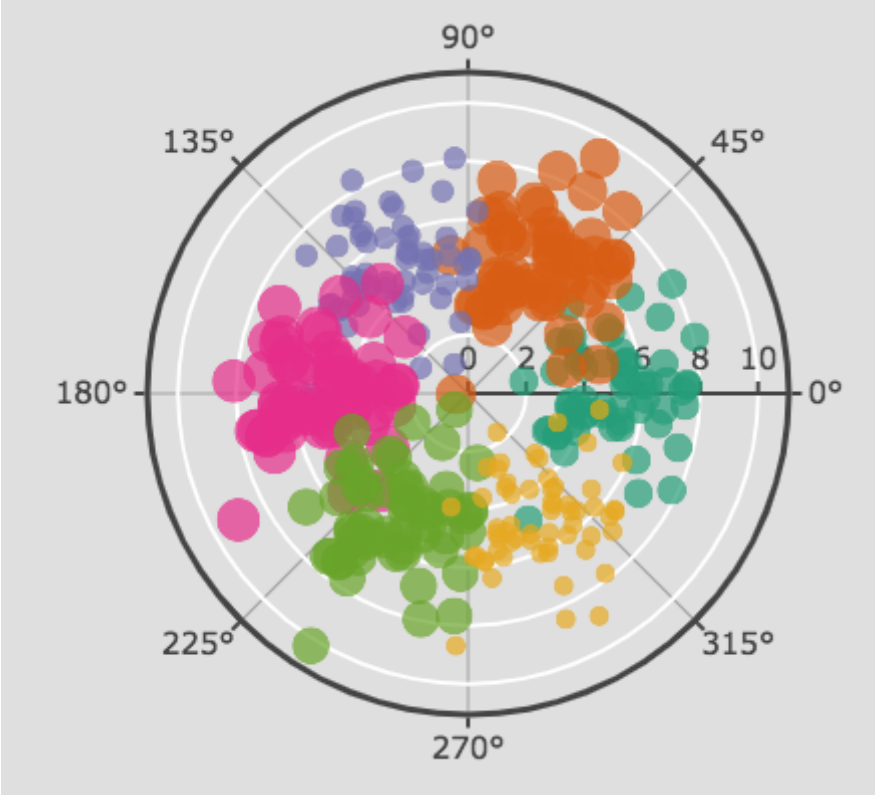

Figure 2: Plot.ly examples showing a Python-created Polar Chart from https://plot.ly/python/polar-chart/. Corresponding data can be linked to the figure and either hosted locally or in an outside repository, using the 'Data Link' capability.

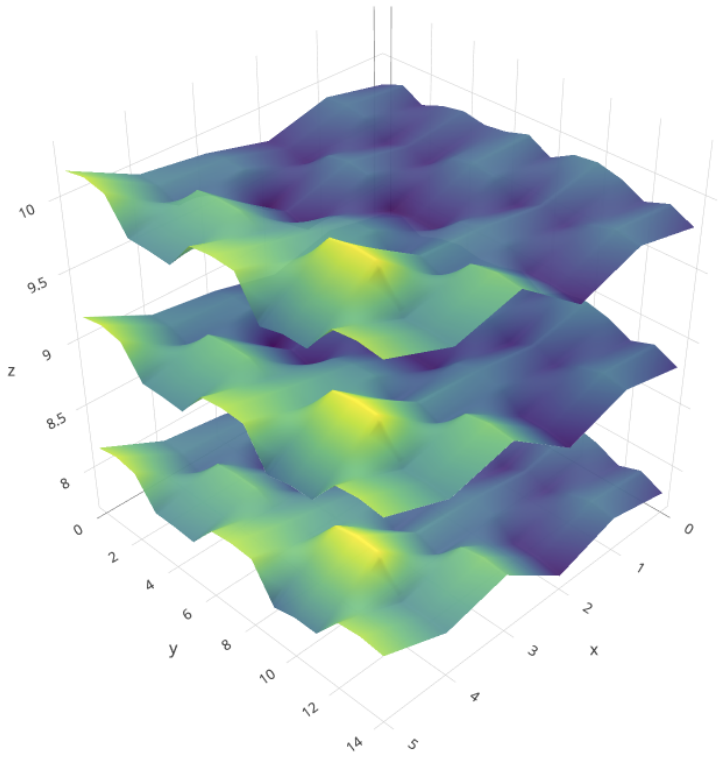

Figure 3: And another Plot.ly example.

Executable Codes

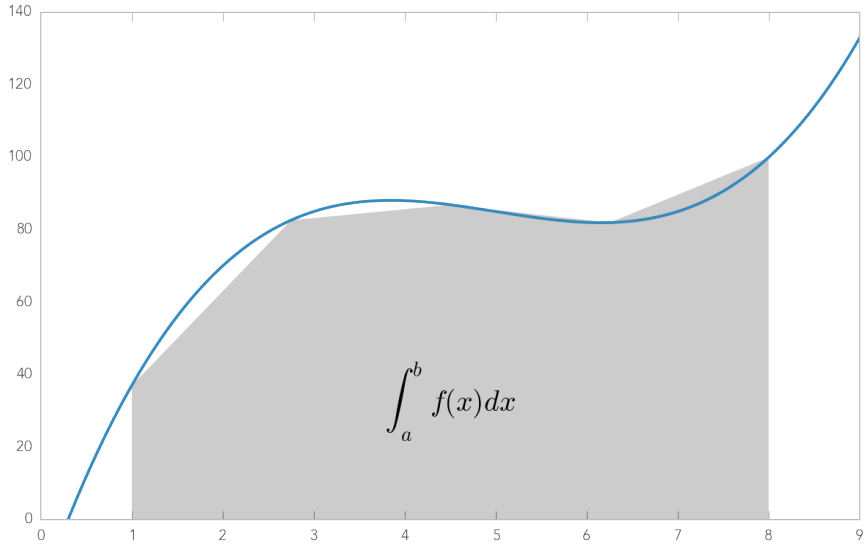

Figure 4: *A simple illustration of the trapezoid rule for definite integration, see section [XXX] in the manuscript.* Here, the code (**Jupyter Notebook hosted locally**) is executed through the icon on the left side of the image. "Executable Figures" are indicated by the </>`Code` icon its top-left side. We can do `R` too!

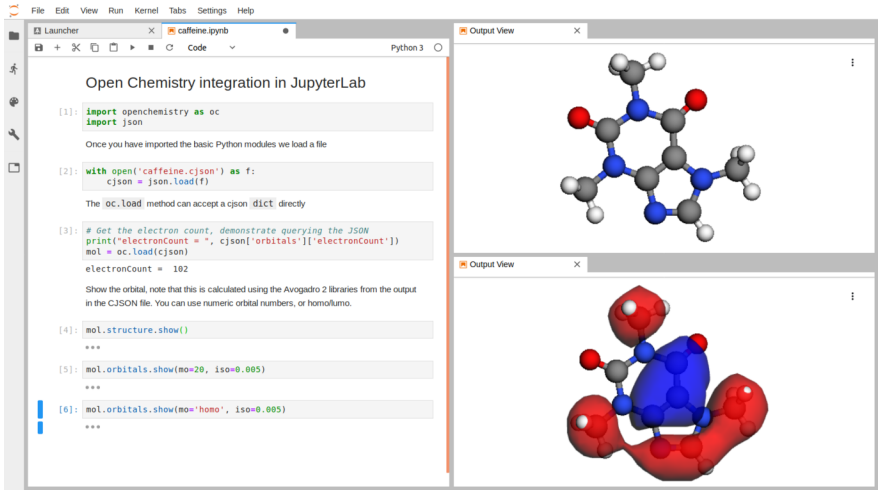

Figure 5: JupyterLab extension allows the visualization of molecular structures in a notebook, with **Binder** used here as external repository of data & code (Accessible via (DataLink)). From (Hanwell et al.).

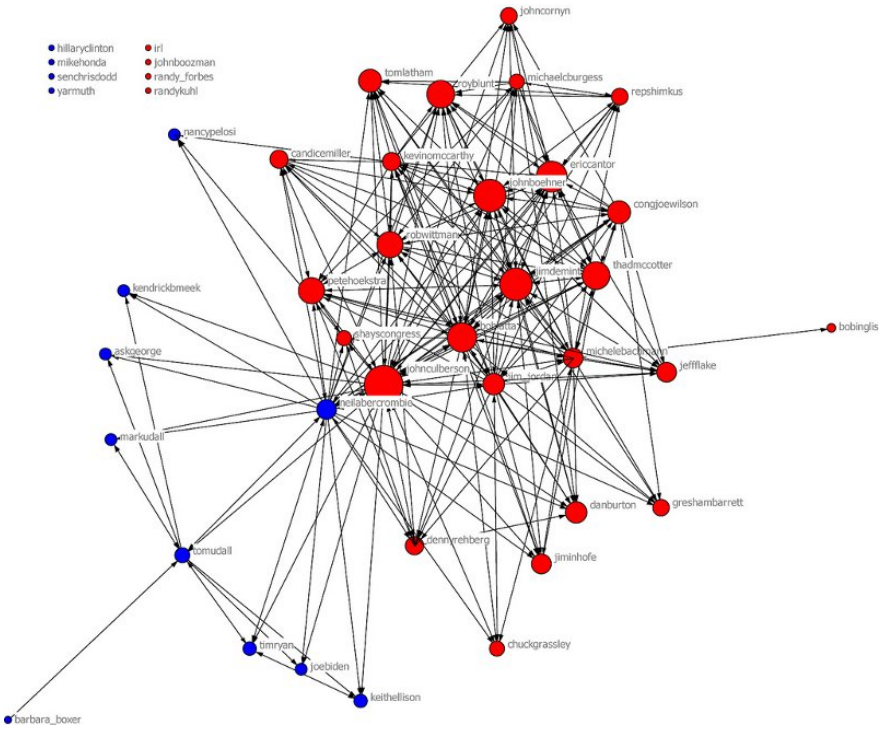

Figure 6: Figure links, via the (Data Link icon) to an executable **CodeOcean** capsule: A Samuel Pottinger (2019) Machine Learning Techniques for Detecting Identifying Linguistic Patterns in the News Media [Source Code]. From (oce).

3D CAD objects

Figure 7: 3D CAD objects can be imported using Java Script modules. Here is an example from 3DViewer.net.

Blender

Figure 8: Standalone HTML5 object from Blender, inserted as interactive figure. Artwork from Marco Squillaci.

References

Inserting an interactive figure. https://support.authorea.com/en-us/article/inserting-an-interactive-figure-y32ne6/. URL https://support.authorea.com/en-us/article/inserting-an-interactive-figure-y32ne6/. Accessed on Thu, September 03, 2020.

Code Ocean. https://codeocean.com/capsule/4002498/tree/v2. URL https://codeocean.com/capsule/4002498/tree/v2. Accessed on Thu, December 03, 2020.

Marcus D Hanwell, Chris Harris, Alessandro Genova, Mojtaba Haghighatlari, Muammar El Khatib, Patrick Avery, Johannes Hachmann, and Wibe Albert de Jong. Open Chemistry, JupyterLab REST and Quantum Chemistry. URL https://doi.org/10.22541%2Fau.158687268.81852407.

Marcus D Hanwell, Chris Harris, Alessandro Genova, Mojtaba Haghighatlari, Muammar El Khatib, Patrick Avery, Johannes Hachmann, and Wibe Albert de Jong. Open Chemistry, JupyterLab REST and Quantum Chemistry. aug 2020. doi: 10.22541/au.158687268.81852407/v2. URL https://doi.org/10.22541%2Fau.158687268.81852407%2Fv2.

Roberto Peverati. Fitting elephants in the density functionals zoo: Statistical criteria for the evaluation of density functional theory methods as a suitable replacement for counting parameters. *International Journal of Quantum Chemistry*, 121(1), jul 2020. doi: 10.1002/qua.26379. URL https://doi.org/10.1002%2Fqua.26379.