

Niraj Nepal <tuq11655@temple.edu>

structure factor: figures and codes

4 messages

Adrienn Ruzsinszky <tuf27796@temple.edu> To: Niraj Kumar Nepal <tug11655@temple.edu> Wed, Feb 5, 2020 at 7:26 PM

Hi Niraj,

I am attaching the material that we discussed today.

The excel file has now five new tabs: the three structure factor Q's

show the spectral analysis for rs=4 with all methods and just for

the three NEOs. The same analysis with the NEOs is repeated for Cs.

The two int structure factors are the integrated S quantities (xc

and correlation energies) for rs=4 and Cs. These last figures correspond

to Figure 2 in John's wavevector analysis paper.

In my notation NEOxc means that we use the x from RPA and c beyond RPA

from NEO.

I am attaching the corresponding codes.(in the integrated S, I am closing the contour for the integral along the imaginary axis taking the real part of khi).

The last attachment is John's paper about the charge density waves.

Good night for now, Adrienn

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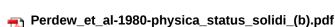
4 attachments

612K

3	plasmon_ 570K	_disp.xlsx
	570K	

\Box	plasmon_	_aısp_	_complex	_struct.i
\Box	plasmon_ 32K			

\Box	plasmon_	_disp_	_complex	_strucfq.f
\Box	22K			



Adrienn Ruzsinszky <tuf27796@temple.edu> To: Niraj Kumar Nepal <tug11655@temple.edu>

Wed, Feb 5, 2020 at 7:47 PM

For rs=4, the "low-density" NEO c should be 0.43 not 0.44. I forgot to correct it in some of the figures. For Cs c=0.44.

Adrienn

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Adrienn Ruzsinszky <tuf27796@temple.edu> To: Niraj Kumar Nepal <tug11655@temple.edu> Wed, Feb 5, 2020 at 7:49 PM

Ooops, it is correct, sorry, Cs NEO c=0.43. Everything is correct as it is. I am getting a little sleepy...

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Niraj Nepal <tug11655@temple.edu> To: Adrienn Ruzsinszky <tuf27796@temple.edu> Wed, Feb 5, 2020 at 8:01 PM

Hi Adrienn,

Thanks, I will look into it.

Best, Niraj

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