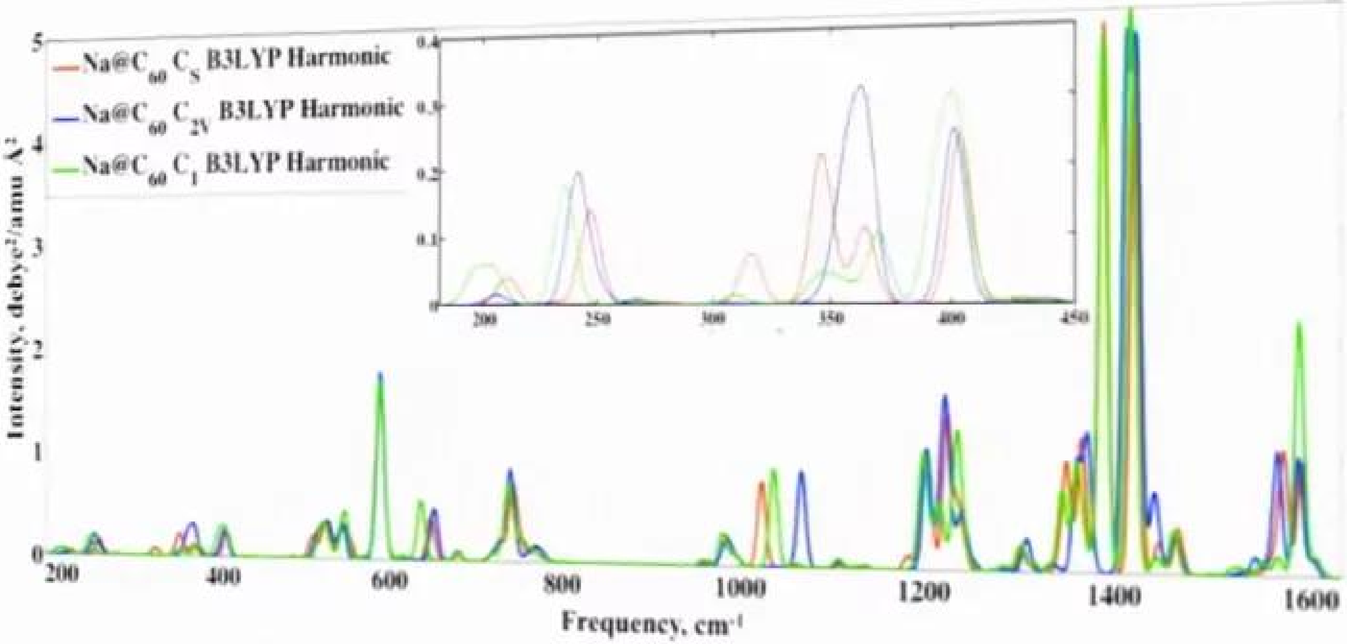
# Structural dependency of IR spectrum



Harmonic IR spectra of Na@$C_{60}$ isomers with $C_1$, $C_{2V}$, and $C_S$ symmetries, obtained with B3LYP/def2-SV(P) level of theory

1
00:00:14,770 --> 00:00:11,240
yeah hi everyone I'm site from you and

2
00:00:18,050 --> 00:00:14,780
our today I'm going to talk about

3
00:00:21,260 --> 00:00:18,060
computational ir spectroscopy for

4
00:00:26,630 --> 00:00:21,270
detection of metal of fullerenes in

5
00:00:31,130 --> 00:00:26,640
space specifically a metal inside c60

6
00:00:34,610 --> 00:00:31,140
and that metal could be lithium sodium

7
00:00:37,340 --> 00:00:34,620
or potassium but generally in a research

8
00:00:43,940 --> 00:00:37,350
group we are trying to answer two

9
00:00:46,190 --> 00:00:43,950
questions what is out there and how it

10
00:00:53,330 --> 00:00:46,200
got formed so today I'm going to talk

11
00:00:55,880 --> 00:00:53,340
about what part here are some outlines

12
00:00:59,750 --> 00:00:55,890
the first I'm going to talk about the

13
00:01:03,080 --> 00:00:59,760

goal of this project and I give you

14
00:01:06,800 --> 00:01:03,090
briefing introduction about fuller is in

15
00:01:09,620 --> 00:01:06,810
space and computation ir spectroscopy

16
00:01:13,190 --> 00:01:09,630
and at the end I show you some

17
00:01:18,740 --> 00:01:13,200
preliminary results and conclusion at

18
00:01:24,740 --> 00:01:18,750
the end so the goal of this project is

19
00:01:29,149 --> 00:01:24,750
to get computationally to obtain ir

20
00:01:33,499 --> 00:01:29,159
spectra for these metal offerings

21
00:01:39,140 --> 00:01:33,509
compound mention but it we have to

22
00:01:41,870 --> 00:01:39,150
include anharmonicity and wide why we

23
00:01:44,960 --> 00:01:41,880
are looking for computational spectra

24
00:01:48,200 --> 00:01:44,970
because these molecules are very hard to

25
00:01:51,679 --> 00:01:48,210
purify and that's why we don't have

26
00:01:53,740 --> 00:01:51,689
experimental data available so we are

27
00:01:58,160 --> 00:01:53,750
trying to make or model it

28
00:02:00,139 --> 00:01:58,170
computationally and the reason we have

29
00:02:06,050 --> 00:02:00,149
to include on harmony city because the

30
00:02:08,930 --> 00:02:06,060
study studies have shown that this into

31
00:02:11,380 --> 00:02:08,940
the interaction between metal and carbon

32
00:02:15,940 --> 00:02:11,390
cage is very weak

33
00:02:18,430 --> 00:02:15,950
and we spare we expect shallow potential

34
00:02:23,110 --> 00:02:18,440
that's why we have to include on harmony

35
00:02:26,559 --> 00:02:23,120
city in our spectrum and for to achieve

36
00:02:28,900 --> 00:02:26,569
these goals we have few steps to follow

37
00:02:33,040 --> 00:02:28,910
first of all we have to locate the

38
00:02:37,800 --> 00:02:33,050

position of that metal atom inside the

39
00:02:42,070 --> 00:02:37,810
cage and find out all the possible

40
00:02:44,710 --> 00:02:42,080
isomers and then get the harmonic

41
00:02:49,050 --> 00:02:44,720
spectra and then to include on harmony

42
00:02:54,460 --> 00:02:49,060
CDV we need to use time dependent and

43
00:02:58,540 --> 00:02:54,470
time independent methods for as for time

44
00:03:02,050 --> 00:02:58,550
independent method we used vs CF or

45
00:03:05,110 --> 00:03:02,060
vibration of self consistent method and

46
00:03:10,750 --> 00:03:05,120
for time-dependent we use molecular

47
00:03:13,509 --> 00:03:10,760
dynamics and this is the telescope this

48
00:03:19,360 --> 00:03:13,519
is called a spitzer and this just

49
00:03:22,020 --> 00:03:19,370
collects information or signals in IR

50
00:03:25,210 --> 00:03:22,030
region infrared region and what

51
00:03:27,160 --> 00:03:25,220
eventually we're going to do is get our

52
00:03:32,350 --> 00:03:27,170
spectra and then compare our results

53
00:03:34,810 --> 00:03:32,360
with the data coming from this telescope

54
00:03:37,690 --> 00:03:34,820
and then if they match we can prove the

55
00:03:43,630 --> 00:03:37,700
presence of metal of fullerenes in the

56
00:03:48,729 --> 00:03:43,640
space and that's how they discovered c60

57
00:03:55,270 --> 00:03:48,739
and CS 70 for the first time in 2010

58
00:04:02,740 --> 00:03:55,280
kami and coworkers modeled see 60 and 70

59
00:04:05,310 --> 00:04:02,750
70 this red line is c 60 they model e

60
00:04:11,220 --> 00:04:05,320
computationally and the blue line boo

61
00:04:14,410 --> 00:04:11,230
spectra is c 70 and then the black

62
00:04:18,789 --> 00:04:14,420
spectra is coming from a spitzer so they

63
00:04:24,490 --> 00:04:18,799

matched it and they proved the presence

64
00:04:30,340 --> 00:04:24,500
of cccc 60 and c 70 in a young

65
00:04:34,870 --> 00:04:30,350
netru nebula so-called tc1 and a few

66
00:04:39,900 --> 00:04:34,880
years later this Duncan co-workers they

67
00:04:42,840 --> 00:04:39,910
found they basically proposed that nom

68
00:04:48,960 --> 00:04:42,850
metal of fullerenes also can be formed

69
00:04:54,490 --> 00:04:48,970
in the same region as easy as easy as

70
00:04:58,420 --> 00:04:54,500
fullerenes and they basically could

71
00:05:03,940 --> 00:04:58,430
synthesize am a sodium inside the cage

72
00:05:08,500 --> 00:05:03,950
of c60 with by under highly energetic

73
00:05:15,610 --> 00:05:08,510
conditions in oxygen and hydrogen rich

74
00:05:17,830 --> 00:05:15,620
and stellar condition and I briefly

75
00:05:20,530 --> 00:05:17,840
talked about my metal but the

76
00:05:26,110 --> 00:05:20,540
methodology I used and computational ir

77
00:05:28,390 --> 00:05:26,120
spectroscopy I need to be faster so the

78
00:05:31,690 --> 00:05:28,400
very first step is getting harmonic

79
00:05:34,210 --> 00:05:31,700
spectra and but then we basically

80
00:05:37,930 --> 00:05:34,220
displays the atoms around their

81
00:05:40,360 --> 00:05:37,940
equilibrium positions and we get the

82
00:05:44,620 --> 00:05:40,370
force constant and calculate the

83
00:05:47,500 --> 00:05:44,630
frequency and this is as I mention this

84
00:05:51,969 --> 00:05:47,510
only includes harmonic frequencies but

85
00:05:56,620 --> 00:05:51,979
we have time independent vibration of

86
00:06:00,190 --> 00:05:56,630
self consistent method we will be sample

87
00:06:03,460 --> 00:06:00,200
energies along the harmonic modes and we

88
00:06:06,430 --> 00:06:03,470

get the vibrational energy levels and

89
00:06:10,830 --> 00:06:06,440
wave functions and we can basically get

90
00:06:15,240 --> 00:06:10,840
the overtones combination bands and

91
00:06:17,830 --> 00:06:15,250
coupling between modes basically and for

92
00:06:21,150 --> 00:06:17,840
time-dependent methods we have molecule

93
00:06:24,130 --> 00:06:21,160
dynamics there are two codes for that

94
00:06:27,010 --> 00:06:24,140
md's molecular dynamics and DRC's

95
00:06:29,950 --> 00:06:27,020
dynamic reaction coordinate this is a

96
00:06:33,970 --> 00:06:29,960
basically classical trajectory based on

97
00:06:37,990 --> 00:06:33,980
the quantum potential energy surface and

98
00:06:39,880 --> 00:06:38,000
be first we have our initial conditions

99
00:06:46,710 --> 00:06:39,890
we have time and energy be putting

100
00:06:50,050 --> 00:06:46,720
system and we use a Fourier transform of

101
00:06:55,440 --> 00:06:50,060
time auto correlation function to go

102
00:06:57,820 --> 00:06:55,450
from time demand to frequency domain and

103
00:07:01,810 --> 00:06:57,830
I know you don't care about these

104
00:07:04,180 --> 00:07:01,820
equations but the first one is the free

105
00:07:08,290 --> 00:07:04,190
and fourier transform for one trajectory

106
00:07:10,780 --> 00:07:08,300
and the last one is for multiple

107
00:07:13,300 --> 00:07:10,790
trajectory when you take average over

108
00:07:16,570 --> 00:07:13,310
multiple trajectories if you have

109
00:07:20,200 --> 00:07:16,580
questions later I can answer but these

110
00:07:29,620 --> 00:07:20,210
are or computational details that we

111
00:07:33,250 --> 00:07:29,630
used again you don't care but tag so

112
00:07:35,830 --> 00:07:33,260
first we got these structures the

113
00:07:38,950 --> 00:07:35,840

isomers of different isomers of sodium

114
00:07:42,190 --> 00:07:38,960
at c60 and then doing future we're

115
00:07:45,760 --> 00:07:42,200
trying to extend it to other metals as

116
00:07:48,760 --> 00:07:45,770
well but this is related to different

117
00:07:51,340 --> 00:07:48,770
symmetries of different positions of

118
00:07:54,250 --> 00:07:51,350
sodium inside the cage with the relative

119
00:07:57,400 --> 00:07:54,260
with their relative energies and this is

120
00:08:00,400 --> 00:07:57,410
the first spectra which is related to

121
00:08:03,390 --> 00:08:00,410
harmonica spectra and the comparison

122
00:08:07,750 --> 00:08:03,400
between those different structures and

123
00:08:12,580 --> 00:08:07,760
as you see here just there is one thing

124
00:08:14,530 --> 00:08:12,590
to mention here that the peaks related

125
00:08:20,260 --> 00:08:14,540
to the movement of sodium inside the

126
00:08:24,430 --> 00:08:20,270
cage it has a redshift for c1 symmetry

127
00:08:28,960 --> 00:08:24,440
and this is where due to the loser bond

128
00:08:30,910 --> 00:08:28,970
of sodium to that structure because of

129
00:08:36,339 --> 00:08:30,920
the position of sodium inside the cage

130
00:08:41,080 --> 00:08:36,349
and here I have a comparison between c63

131
00:08:43,750 --> 00:08:41,090
sixty- and sodium at c60 c6 he has only

132
00:08:45,530 --> 00:08:43,760
four fundamental piece but when we have

133
00:08:47,360 --> 00:08:45,540
c 6 t minus did

134
00:08:49,910 --> 00:08:47,370
the extra electron can which has a

135
00:08:54,249 --> 00:08:49,920
resonance inside the cage can break the

136
00:09:00,710 --> 00:08:54,259
symmetry and we have much more peaks but

137
00:09:04,249 --> 00:09:00,720
you can see the peaks for the blue sorry

138
00:09:07,309 --> 00:09:04,259

the red peaks and the yellow peaks are

139
00:09:11,319 --> 00:09:07,319
matched because we trying to show here

140
00:09:14,540 --> 00:09:11,329
that that extra electron from sodium

141
00:09:17,569 --> 00:09:14,550
radical actually transfers to the cage

142
00:09:19,790 --> 00:09:17,579
and does the same thing as that minus

143
00:09:23,090 --> 00:09:19,800
electron that the extra extra electron

144
00:09:26,090 --> 00:09:23,100
is 60 minus and we have basically the

145
00:09:28,490 --> 00:09:26,100
same peaks except for some extra piece

146
00:09:31,069 --> 00:09:28,500
for sodium acetate is equal and that's

147
00:09:34,670 --> 00:09:31,079
due to the movement of sodium inside the

148
00:09:40,329 --> 00:09:34,680
cage and this is the last result I've

149
00:09:42,530 --> 00:09:40,339
I've got so far for hall which is

150
00:09:45,829 --> 00:09:42,540
comparison between harmonic and on a

151
00:09:50,569 --> 00:09:45,839
harmonic which on harmonic is coming

152
00:09:54,019 --> 00:09:50,579
from vs CF and basically you see here

153
00:09:59,629 --> 00:09:54,029
you see a red shift for on harmonic

154
00:10:06,439 --> 00:09:59,639
Peaks compared to harmonic ones for from

155
00:10:08,980 --> 00:10:06,449
the vs CF met and we also try to ok we

156
00:10:13,370 --> 00:10:08,990
also try to use model molecular dynamics

157
00:10:16,699 --> 00:10:13,380
and first for a simple molecule like

158
00:10:22,009 --> 00:10:16,709
water and that showed us this and not

159
00:10:28,179 --> 00:10:22,019
only can provide us harmonic or normal

160
00:10:31,040 --> 00:10:28,189
modes but also can give us overtones and

161
00:10:35,000 --> 00:10:31,050
overtones and combination bands as you

162
00:10:37,910 --> 00:10:35,010
see here but then we apply this in our

163
00:10:41,150 --> 00:10:37,920

system we could get only lower

164
00:10:43,069 --> 00:10:41,160
frequencies but not higher ones and we

165
00:10:46,819 --> 00:10:43,079
think it's due to the fact that we only

166
00:10:51,199 --> 00:10:46,829
used one trajectory not multiple ones so

167
00:10:55,449 --> 00:10:51,209
we are trying future to use multiple and

168
00:10:58,460 --> 00:10:55,459
take the average over and as a results

169
00:11:00,890 --> 00:10:58,470
ir spectra for these compounds

170
00:11:04,070 --> 00:11:00,900
as I mentioned are very structure

171
00:11:06,500 --> 00:11:04,080
structure of dependent and on one on

172
00:11:09,800 --> 00:11:06,510
harmonic frequencies show the redshift

173
00:11:13,640 --> 00:11:09,810
compared to harmonic one and in future

174
00:11:16,820 --> 00:11:13,650
in order to sample a complete the

175
00:11:19,940 --> 00:11:16,830
spectra we need to first of all include

176
00:11:25,490 --> 00:11:19,950
couplings between modes and also we need

177
00:11:29,540 --> 00:11:25,500
to get put higher temperature or system

178
00:11:31,700 --> 00:11:29,550
and also we need to consider multiple

179
00:11:34,340 --> 00:11:31,710
trajectory instead of one and then we

180
00:11:47,420 --> 00:11:34,350
can extend our work to other method of

181
00:11:50,860 --> 00:11:47,430
fullerenes thank you okay thank you very

182
00:11:52,970 --> 00:11:50,870
much for our presentation I saw you have

183
00:11:59,420 --> 00:11:52,980
different entries for turbulent

184
00:12:01,760 --> 00:11:59,430
symmetries of metal at c60 it is as any

185
00:12:04,370 --> 00:12:01,770
I see your connections to differ

186
00:12:09,830 --> 00:12:04,380
energies barriers for this different

187
00:12:13,730 --> 00:12:09,840
symmetry oh yes yes I didn't do I've

188
00:12:15,710 --> 00:12:13,740

been there is they have different

189
00:12:18,290 --> 00:12:15,720
energies but we don't know about the

190
00:12:27,470 --> 00:12:18,300
barrier that as I shoot here in this

191
00:12:30,920 --> 00:12:27,480
slide oh okay yes first not yeah yeah

192
00:12:33,860 --> 00:12:30,930
and the energy difference so if there

193
00:12:37,640 --> 00:12:33,870
are relative energies but if this is 0

194
00:12:40,610 --> 00:12:37,650
this is 72 this is 73 but this is what

195
00:12:50,600 --> 00:12:40,620
we have found so far they might be more

196
00:13:00,079 --> 00:12:57,769
I guess I was just wondering um so what

197
00:13:02,690 --> 00:13:00,089
is the nature of the coordination or the

198
00:13:06,620 --> 00:13:02,700
bonding of the metal within the cage is

199
00:13:11,449 --> 00:13:06,630
it ok so the global minimum of which

200
00:13:14,300 --> 00:13:11,459
that we have found so far is the sodium

201
00:13:17,630 --> 00:13:14,310
is in between it's closer to the wall

202
00:13:20,990 --> 00:13:17,640
and it is in between pentagons and

203
00:13:25,310 --> 00:13:21,000
hexagons that's the global minima we

204
00:13:28,160 --> 00:13:25,320
have found so far but I'm doing more

205
00:13:40,880 --> 00:13:28,170
calculations to find more structures ok

206
00:13:45,100 --> 00:13:40,890
yeah I'm just wondering how you did the

207
00:13:47,960 --> 00:13:45,110
exploration of the minimum

208
00:13:53,060 --> 00:13:47,970
configurations of sodium in the bucket

209
00:14:00,019 --> 00:13:53,070
ball ok so first I picked some

210
00:14:04,639 --> 00:14:00,029
symmetries c1 c2 VCS c5 ec3v and then I

211
00:14:06,860 --> 00:14:04,649
did geometry optimization I found the

212
00:14:08,900 --> 00:14:06,870
structures and the idea the Haitian

213
00:14:12,530 --> 00:14:08,910

calculation at the top of that if they

214
00:14:15,170 --> 00:14:12,540
have imaginary frequencies I distort

215
00:14:21,680 --> 00:14:15,180
them along that imaginary frequency to

216
00:14:26,150 --> 00:14:21,690
get equilibrium or actual minima but so

217
00:14:29,720 --> 00:14:26,160
far only these three structures have no